



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 10:45 PM JST

PDB ID : 7V32 / pdb_00007v32
EMDB ID : EMD-31650
Title : Deactive state complex I from rotenone dataset
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-08-10
Resolution : 3.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

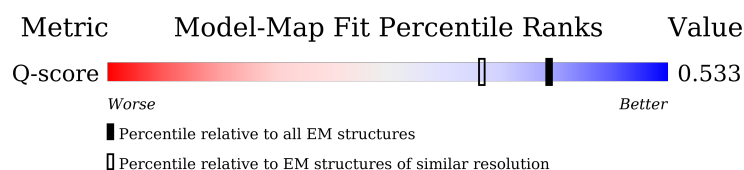
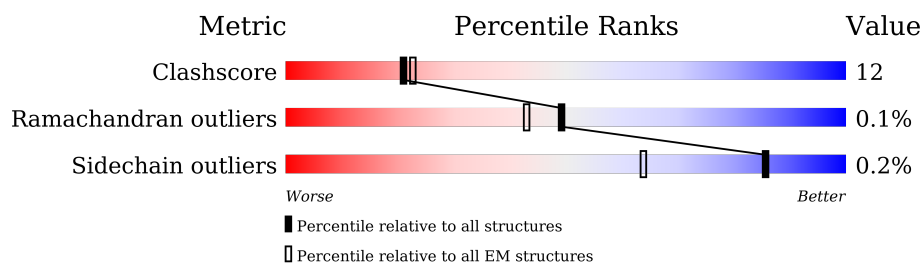
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	431	
2	B	176	
3	C	156	
4	E	115	

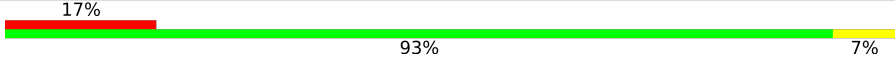
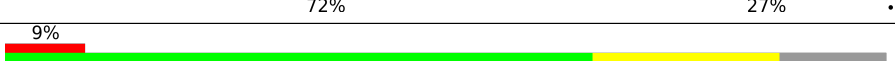
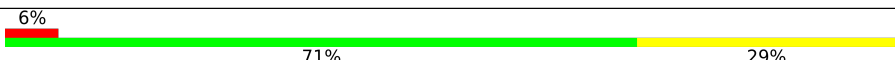
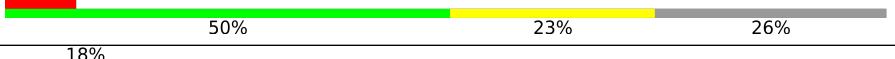
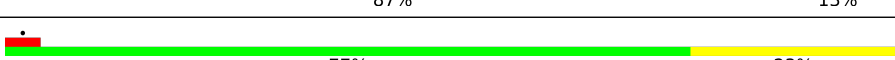
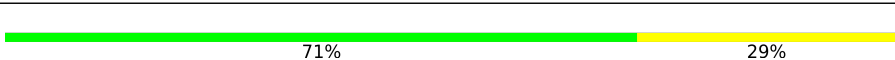
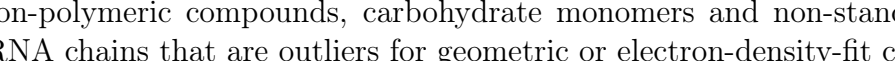
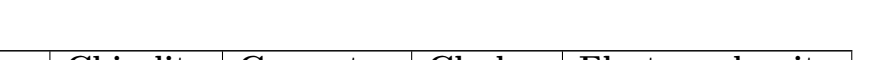
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Mol	Chain	Length	Quality of chain
5	F	86	
6	G	88	
6	X	88	
7	H	112	
8	I	112	
9	J	341	
10	K	42	
11	L	125	
12	M	690	
13	N	144	
14	O	217	
15	P	208	
16	Q	430	
17	S	70	
18	T	96	
19	U	83	
20	V	140	
21	W	142	
22	Y	70	
23	Z	84	
24	a	140	
25	b	126	
26	c	156	
27	d	175	
28	e	107	

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Mol	Chain	Length	Quality of chain
29	f	42	
30	g	121	
31	h	105	
32	i	347	
33	j	113	
34	k	98	
35	l	603	
36	m	175	
37	n	56	
38	o	128	
39	p	178	
40	r	459	
41	s	318	
42	u	171	
43	v	131	
44	w	320	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	SF4	A	501	-	-	X	-
47	PEE	l	704	-	-	X	-
47	PEE	m	201	-	-	X	-
53	CDL	a	201	-	-	X	-
56	ADP	w	401	-	-	X	-

2 Entry composition [i](#)

There are 56 unique types of molecules in this entry. The entry contains 66596 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	431	Total	C	N	O	S	0	0
			3318	2095	591	612	20		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	176	Total	C	N	O	S	0	0
			1412	887	243	269	13		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	156	Total	C	N	O	S	0	0
			1248	794	227	213	14		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	115	Total	C	N	O	S	0	0
			971	619	179	168	5		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	86	Total	C	N	O	S	0	0
			691	434	129	126	2		

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total	C	N	O	S	0	0
			664	425	102	132	5		
6	X	88	Total	C	N	O	S	0	0
			693	445	102	141	5		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	112	Total	C	N	O	S	0	0
			910	588	154	165	3		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	97	Total	C	N	O	S	0	0
			780	491	147	139	3		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	297	Total	C	N	O	S	0	0
			2352	1511	421	412	8		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	42	Total	C	N	O	S	0	0
			355	219	67	68	1		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	125	Total	C	N	O	S	0	0
			1016	642	181	190	3		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	690	Total	C	N	O	S	0	0
			5293	3319	923	1012	39		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	144	Total	C	N	O	S	0	0
			1204	770	218	212	4		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	217	Total	C	N	O	S	0	0
			1660	1057	281	312	10		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	208	Total	C	N	O	S	0	0
			1738	1124	298	314	2		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	419	Total	C	N	O	S	0	0
			3377	2162	578	613	24		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	70	Total	C	N	O	S	0	0
			567	364	104	94	5		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	96	Total	C	N	O	S	0	0
			741	452	140	146	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	83	Total	C	N	O	S	0	0
			643	417	110	115	1		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	140	Total	C	N	O	S	0	0
			1021	651	174	190	6		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	142	Total	C	N	O	S	0	0
			1167	752	200	206	9		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	70	Total	C	N	O	S	0	0
			600	393	98	108	1		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	84	Total	C	N	O	S	0	0
			674	437	116	120	1		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	140	Total	C	N	O	S	0	0
			1161	760	199	199	3		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	103	Total	C	N	O	S	0	0
			879	573	158	147	1		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	156	Total	C	N	O	S	0	0
			1315	853	213	241	8		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	175	Total	C	N	O	S	0	0
			1461	916	265	272	8		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	107	Total	C	N	O	S	0	0
			890	568	145	173	4		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	42	Total	C	N	O	0	0
			342	225	58	59		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	121	Total	C	N	O	S	0	0
			1000	650	173	171	6		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	105	Total	C	N	O	S	0	0
			867	550	161	150	6		

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	347	Total	C	N	O	S	0	0
			2710	1782	420	462	46		

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	99	Total	C	N	O	S	0	0
			800	545	118	132	5		

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	k	98	Total	C	N	O	S	0	0
			748	493	113	128	14		

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	603	Total	C	N	O	S	0	0
			4785	3173	741	820	51		

- Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	129	Total	C	N	O	S	0	0
			951	637	138	168	8		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	56	Total	C	N	O	S	0	0
			456	295	83	77	1		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit

4.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	o	128	Total	C	N	O	0	0
			1062	691	182	189		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	178	Total	C	N	O	S	0	0
			1534	982	279	265	8		

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	r	459	Total	C	N	O	S	0	0
			3631	2412	572	609	38		

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	303	Total	C	N	O	S	0	0
			2394	1607	369	397	21		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	u	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	124	Total	C	N	O	S	0	0
			992	622	180	181	9		

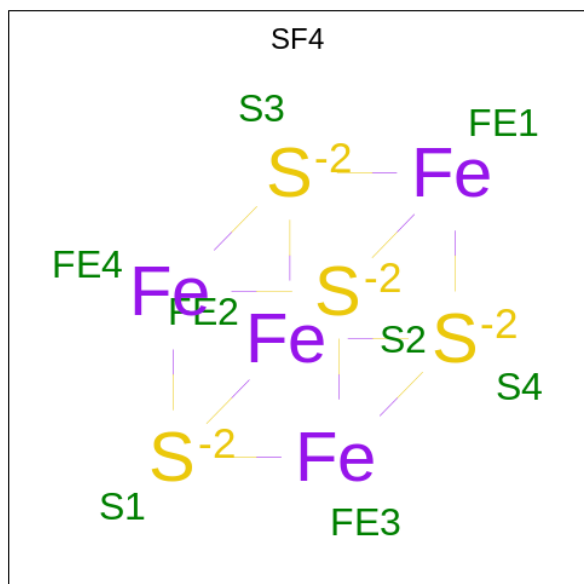
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	1	MYR	-	acetylation	UNP F1SCH1

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

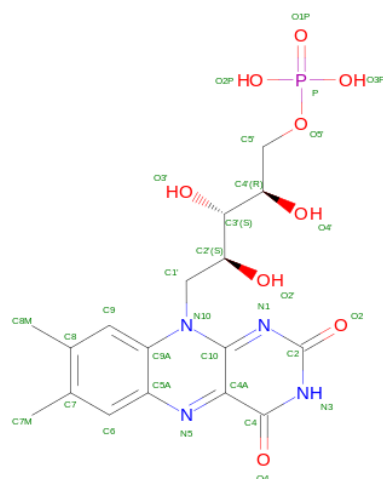
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2586	1646	439	491	10		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



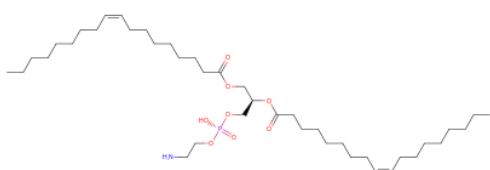
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 47 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



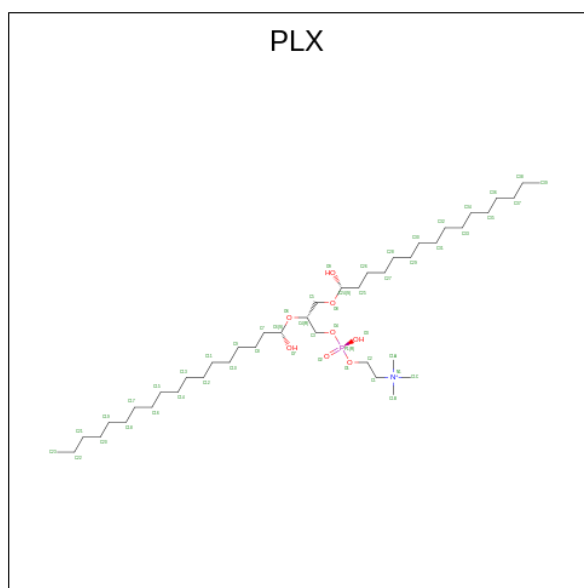
Mol	Chain	Residues	Atoms					AltConf
47	B	1	Total 51	C 41	N 1	O 8	P 1	0
47	U	1	Total 51	C 41	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
47	i	1	Total	C	N	O	P	0
			47	37	1	8	1	
47	j	1	Total	C	N	O	P	0
			47	37	1	8	1	
47	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
47	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
47	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
47	r	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 48 is (9R,11S)-9-([[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



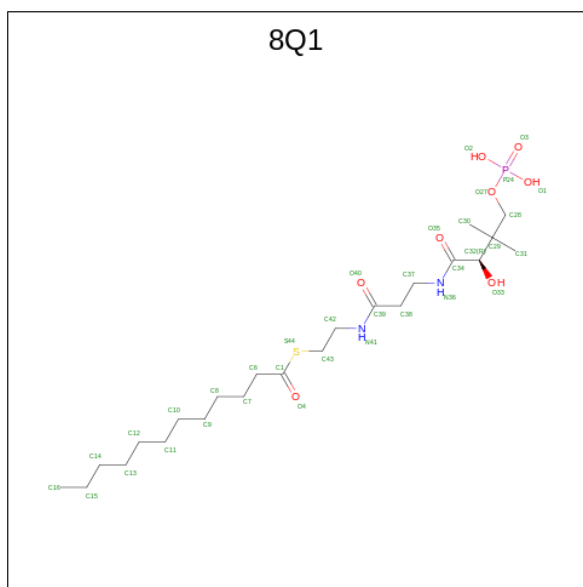
Mol	Chain	Residues	Atoms					AltConf
48	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	j	1	Total	C	N	O	P	0
			52	42	1	8	1	

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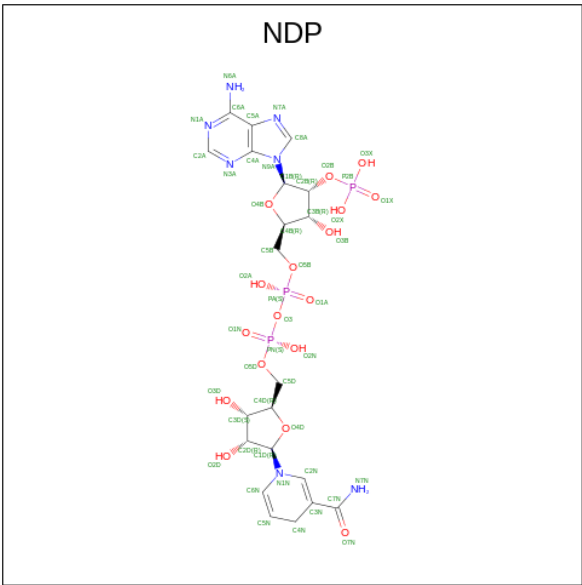
Mol	Chain	Residues	Atoms					AltConf
48	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 49 is S-[2-(N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl)amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



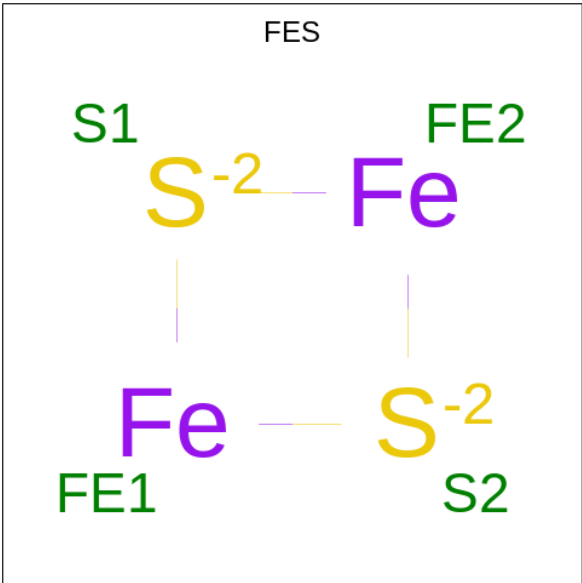
Mol	Chain	Residues	Atoms						AltConf
49	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
49	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 50 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
50	J	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 51 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).

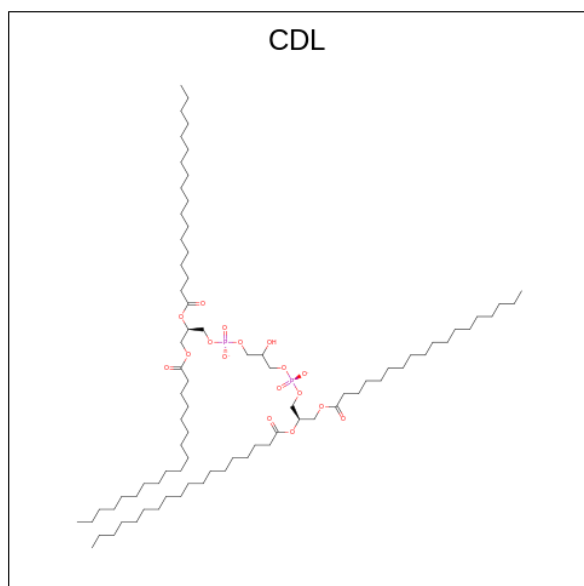


Mol	Chain	Residues	Atoms			AltConf
51	M	1	Total	Fe	S	0
			4	2	2	
51	O	1	Total	Fe	S	0
			4	2	2	

- Molecule 52 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
52	M	1	Total	Mg	0
			1	1	

- Molecule 53 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).

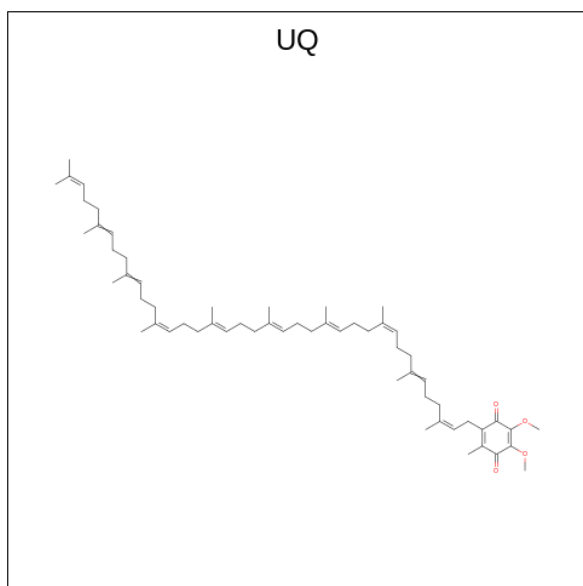


Mol	Chain	Residues	Atoms				AltConf
53	N	1	Total	C	O	P	0
			51	32	17	2	
53	a	1	Total	C	O	P	0
			91	72	17	2	
53	g	1	Total	C	O	P	0
			100	81	17	2	
53	i	1	Total	C	O	P	0
			66	47	17	2	
53	l	1	Total	C	O	P	0
			99	80	17	2	
53	l	1	Total	C	O	P	0
			100	81	17	2	
53	n	1	Total	C	O	P	0
			78	59	17	2	

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

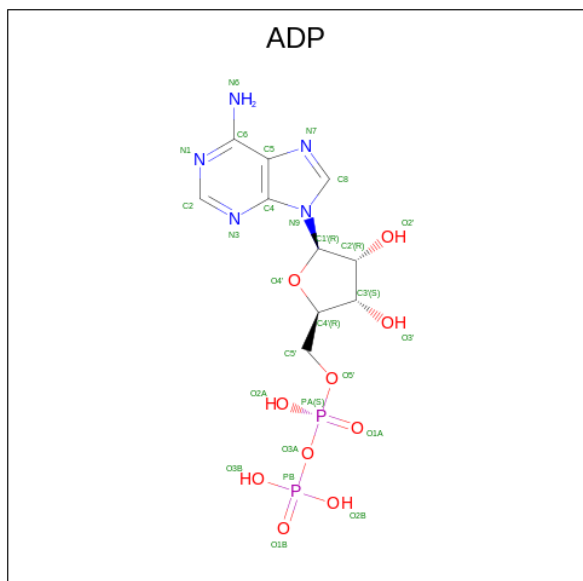
Mol	Chain	Residues	Atoms		AltConf
54	T	1	Total	Zn	0
			1	1	

- Molecule 55 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: C₅₉H₉₀O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
55	s	1	Total	C	O	0
			28	24	4	

- Molecule 56 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

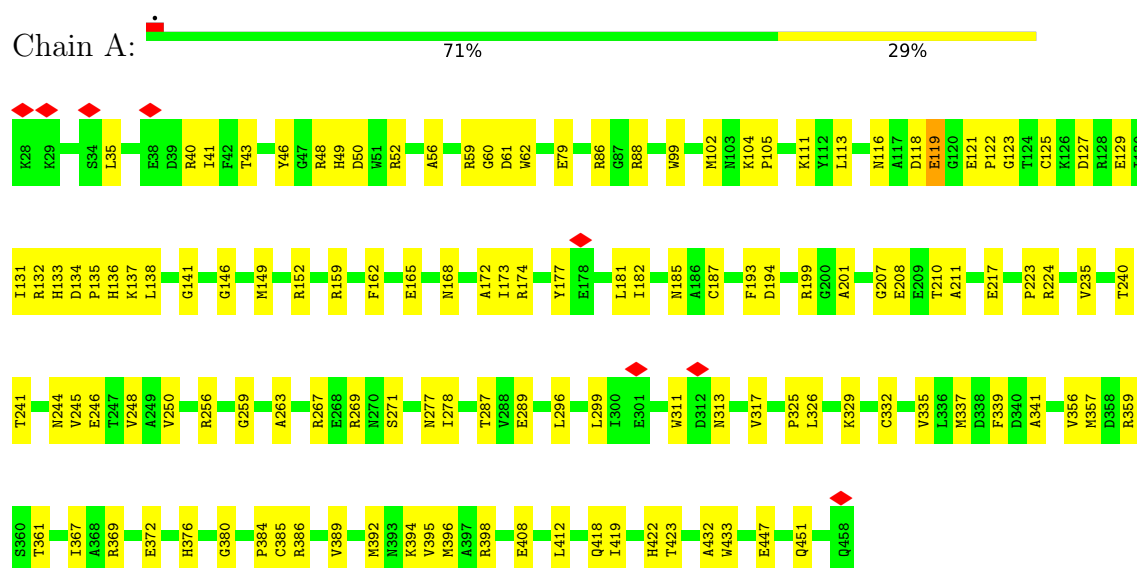


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
56	w	1	27	10	5	10	2	0

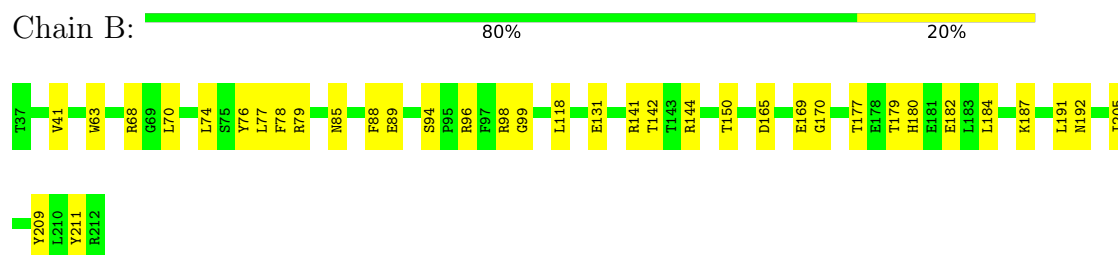
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

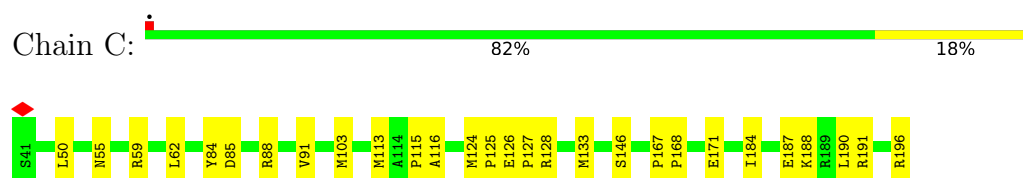
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



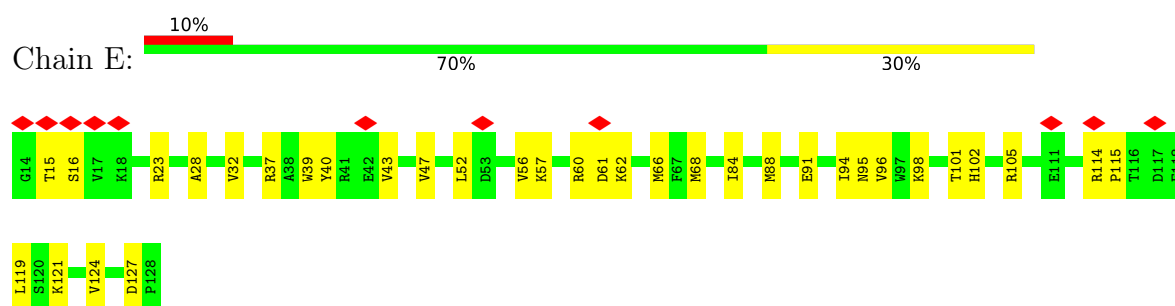
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



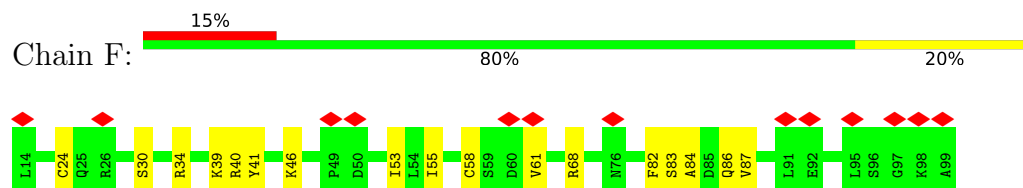
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



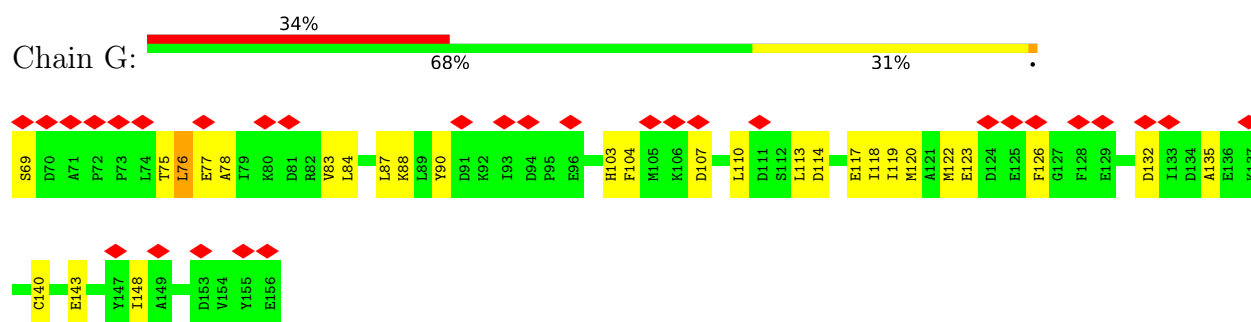
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



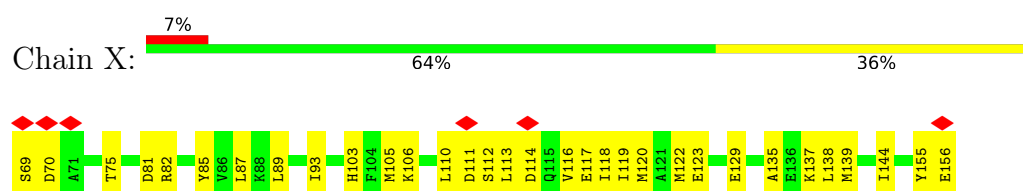
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



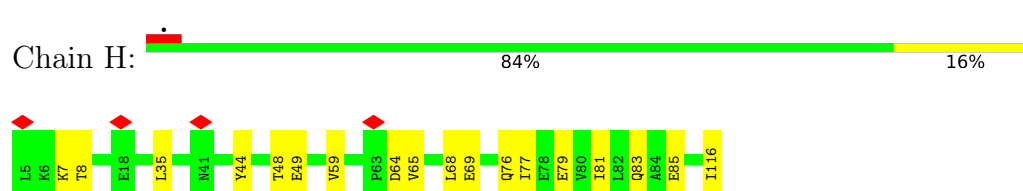
- Molecule 6: Acyl carrier protein, mitochondrial



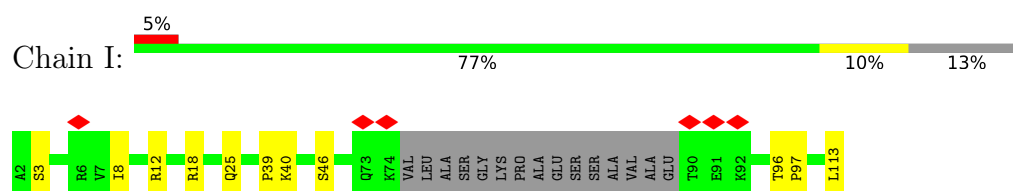
- Molecule 6: Acyl carrier protein, mitochondrial



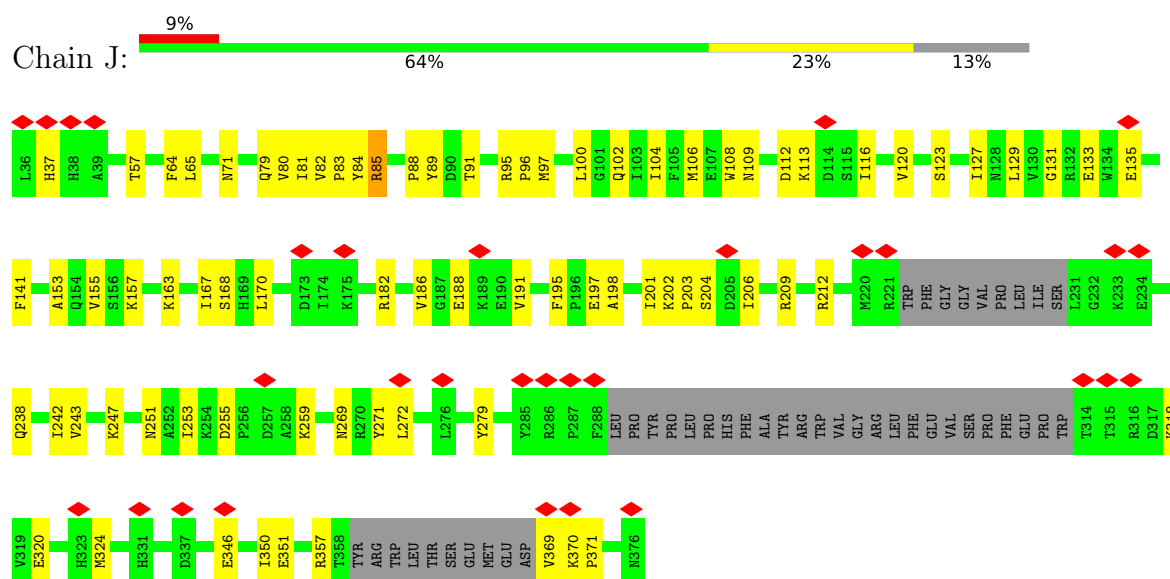
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



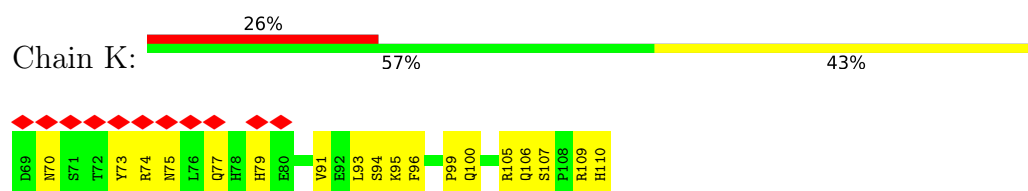
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



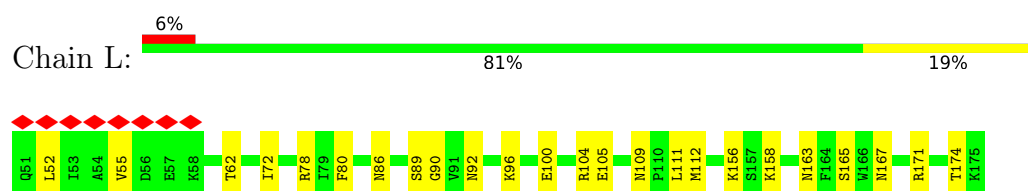
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



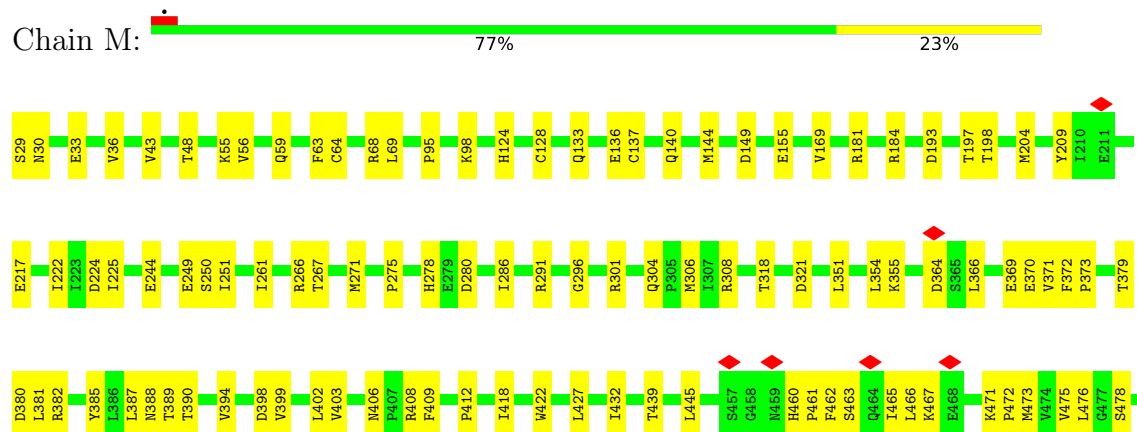
- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

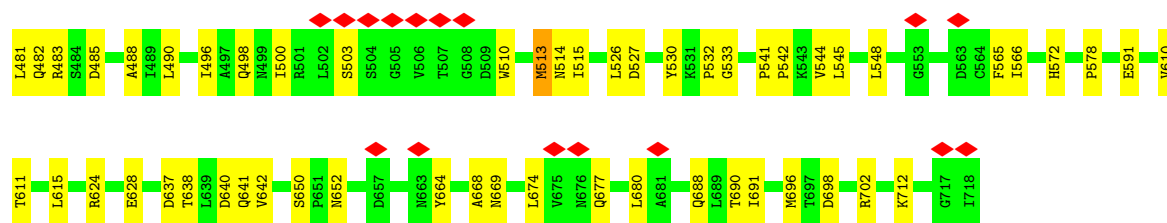


- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

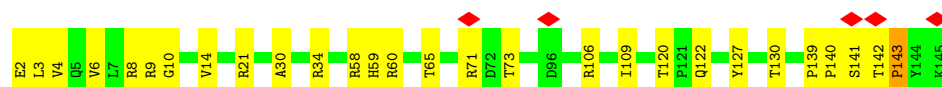
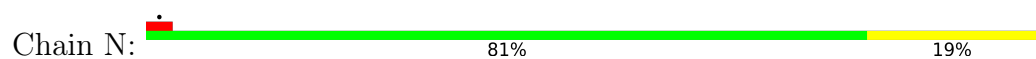


- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

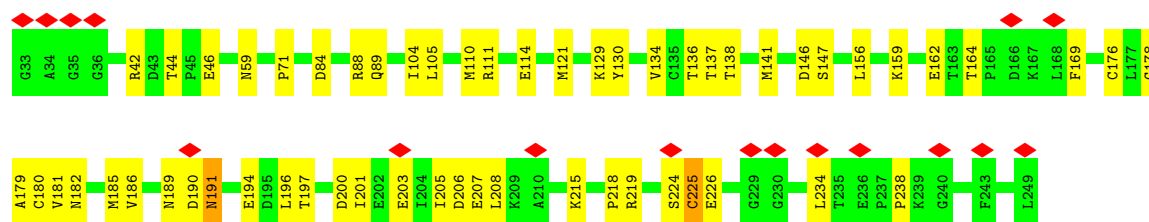
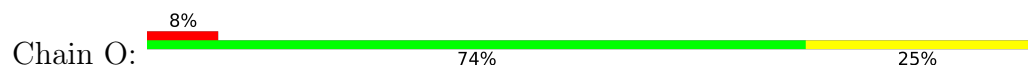




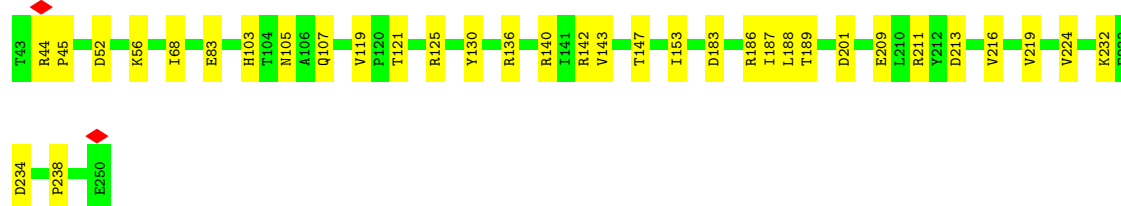
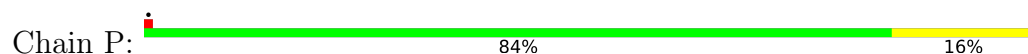
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



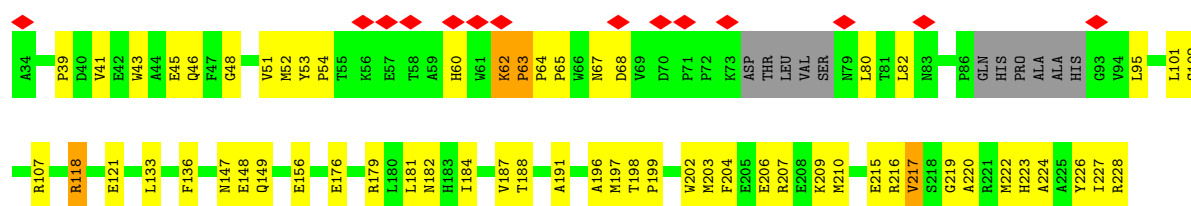
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

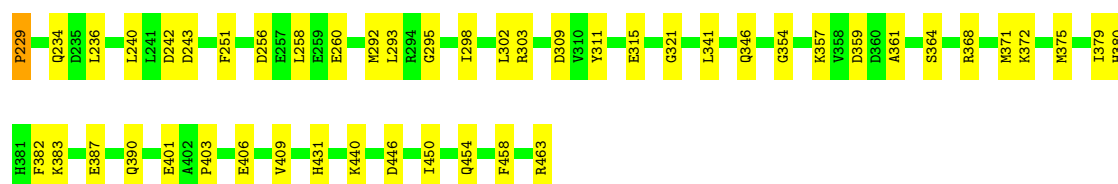


- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

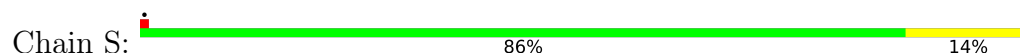


- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

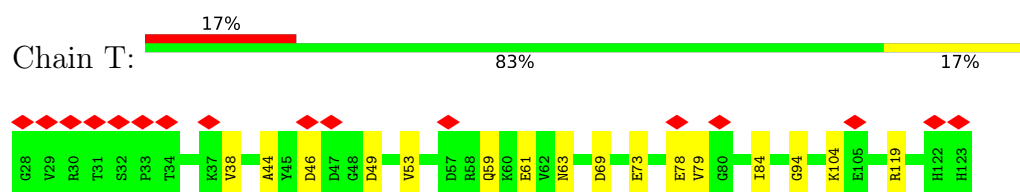




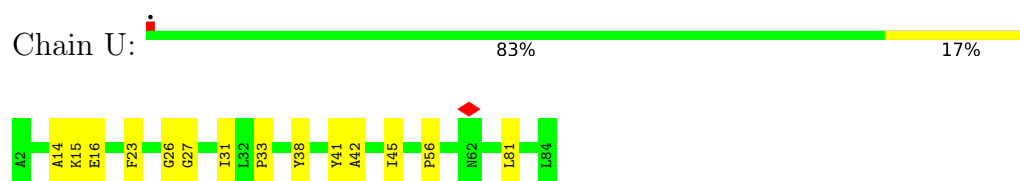
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



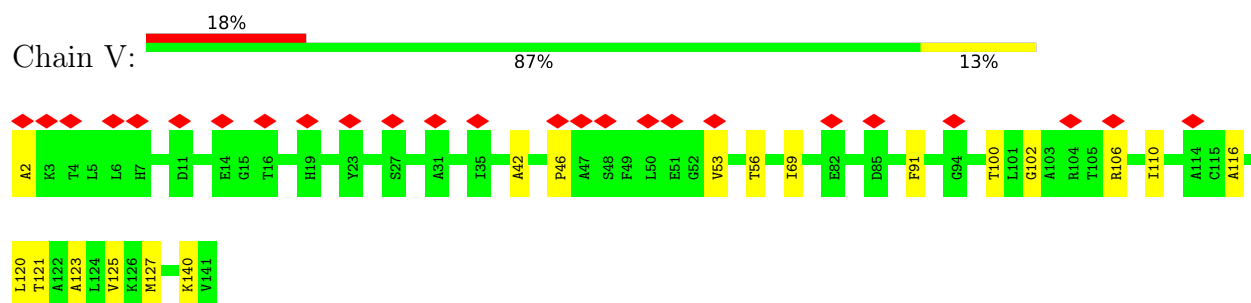
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



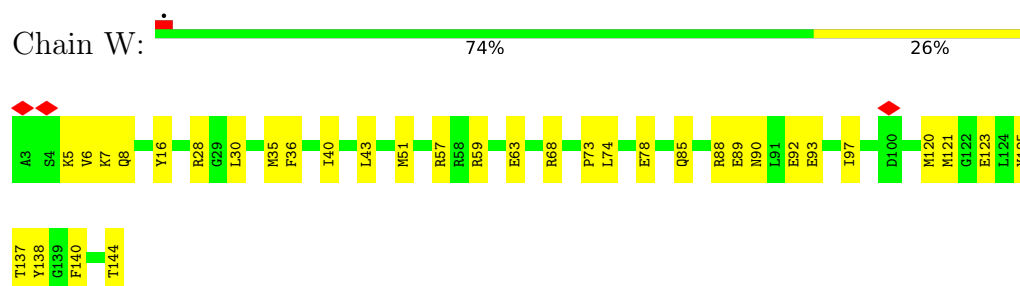
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



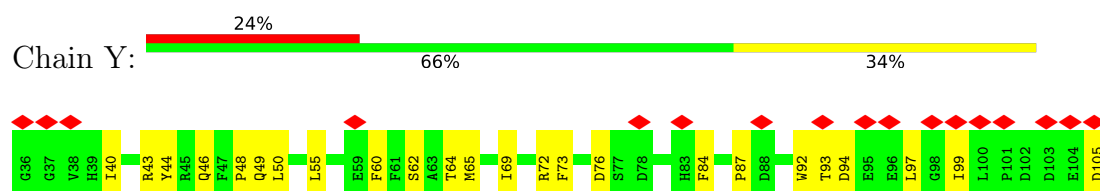
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



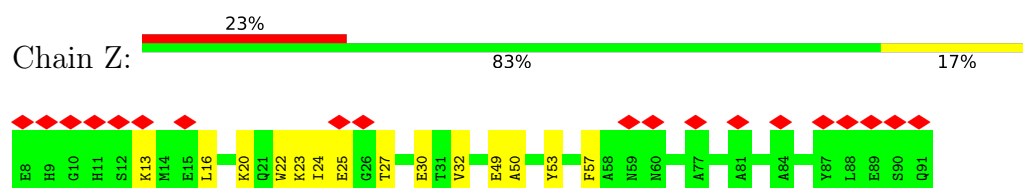
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



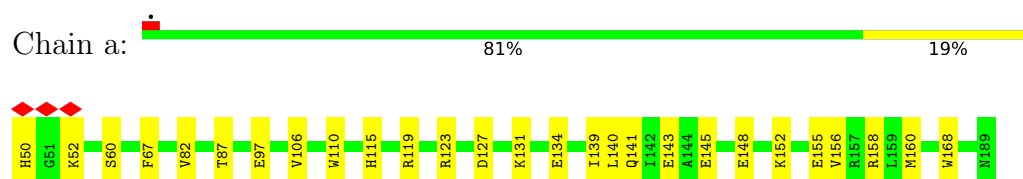
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



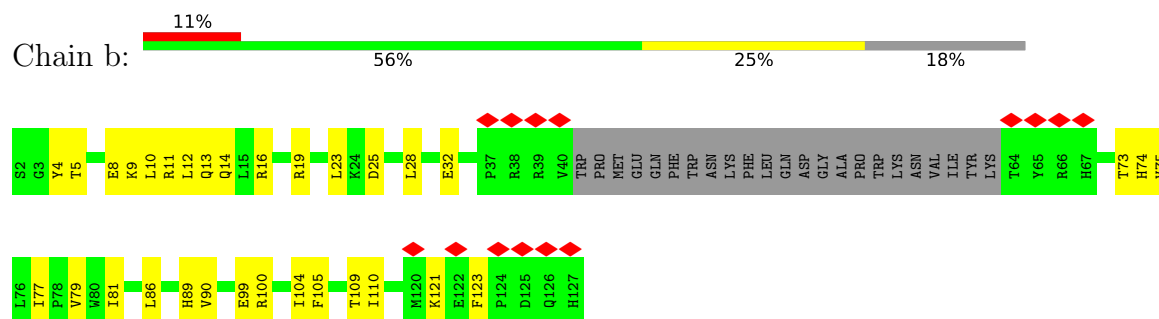
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



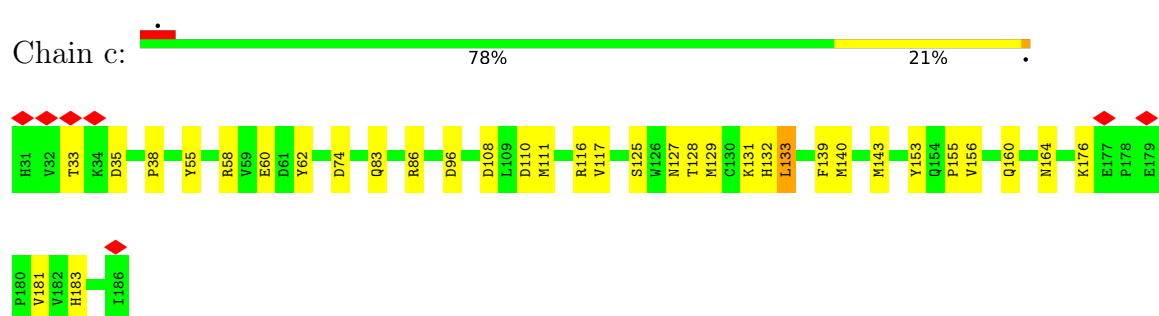
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



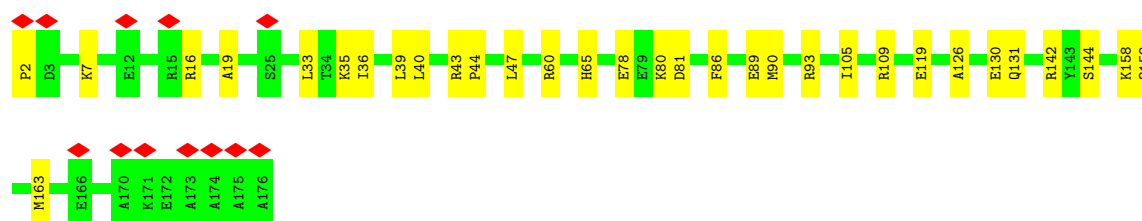
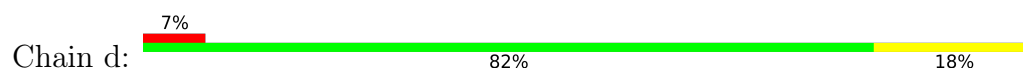
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



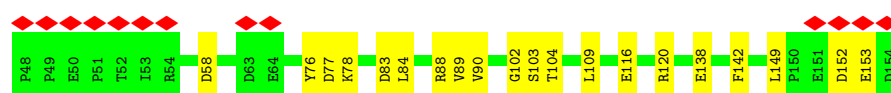
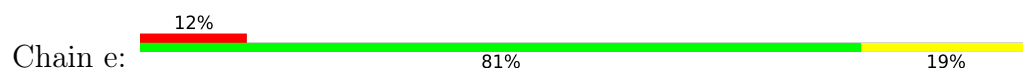
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



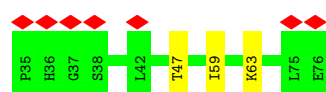
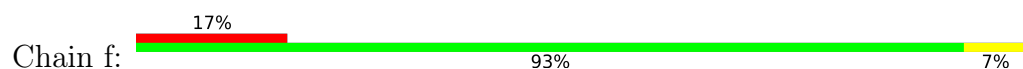
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



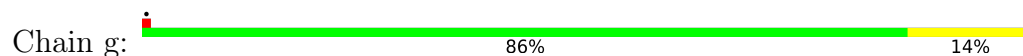
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



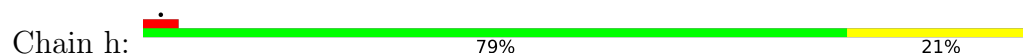
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

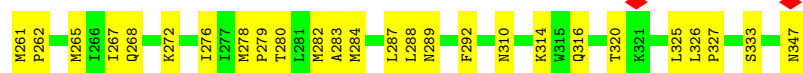


- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

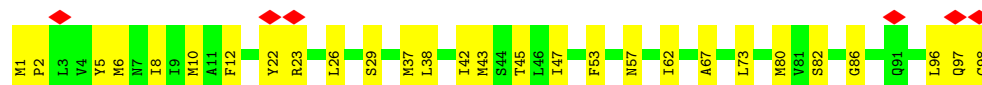




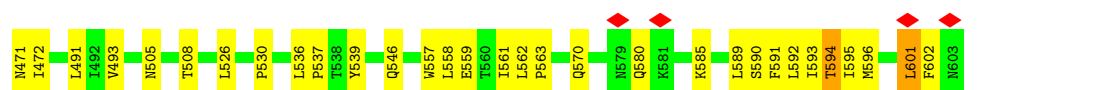
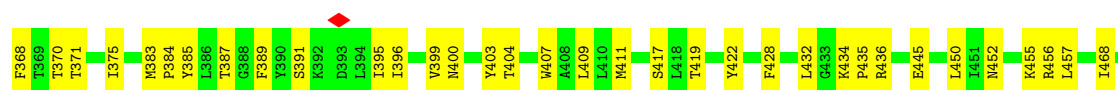
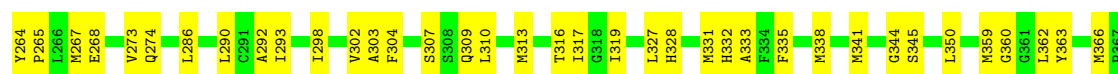
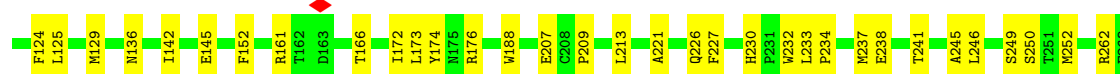
• Molecule 33: NADH-ubiquinone oxidoreductase chain 3



• Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

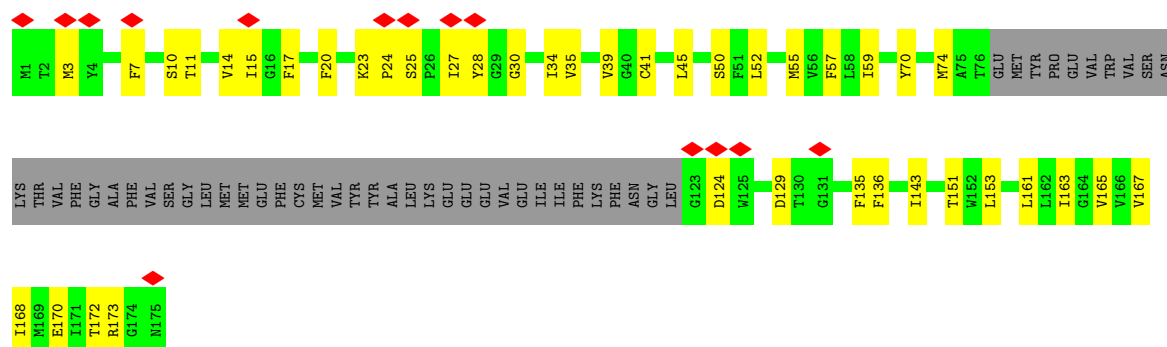


• Molecule 35: NADH-ubiquinone oxidoreductase chain 5



• Molecule 36: NADH-ubiquinone oxidoreductase chain 6

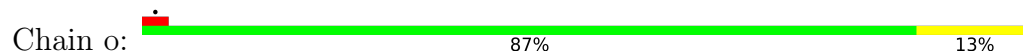




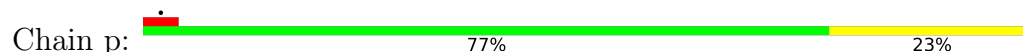
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



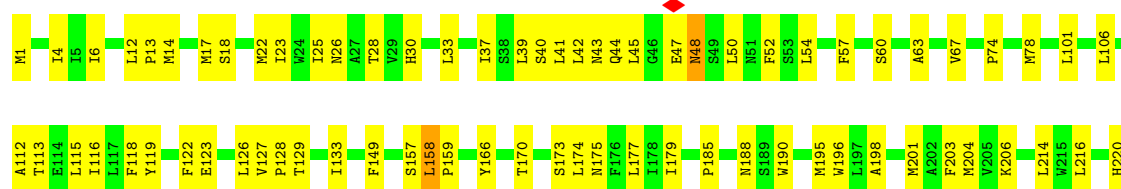
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

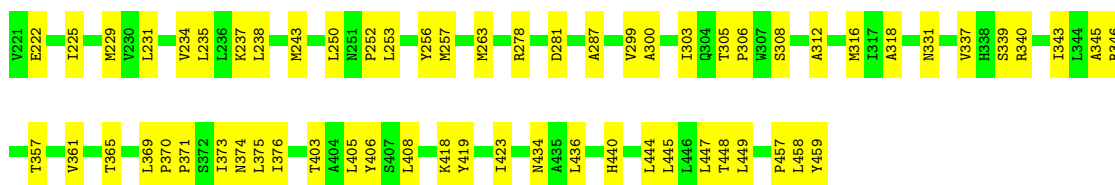


- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

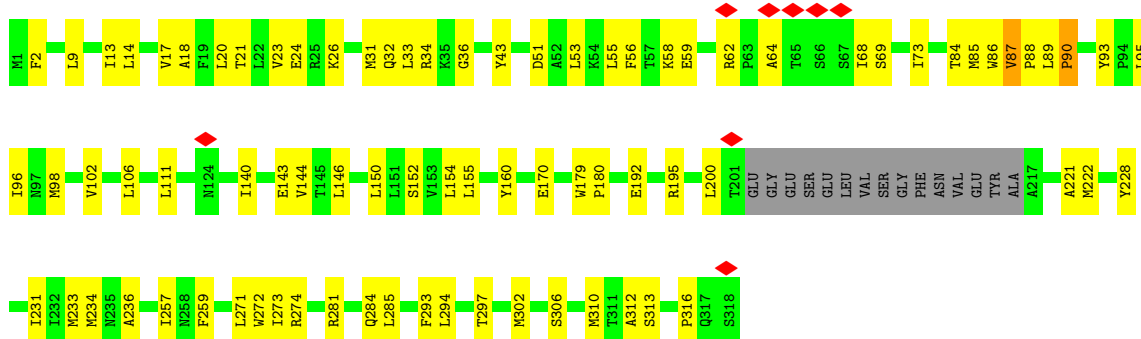


- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

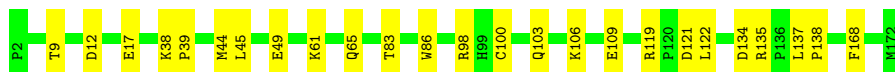
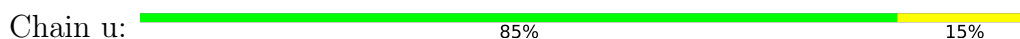




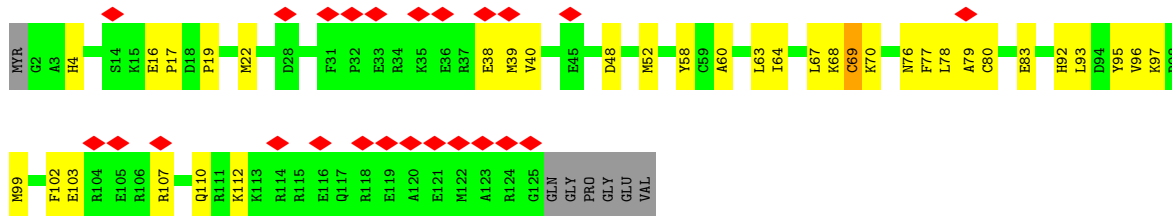
• Molecule 41: NADH-ubiquinone oxidoreductase chain 1



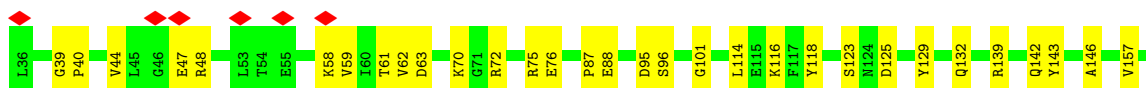
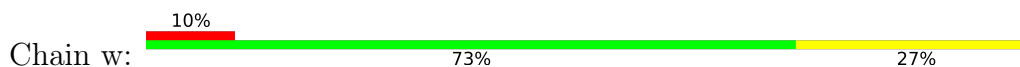
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

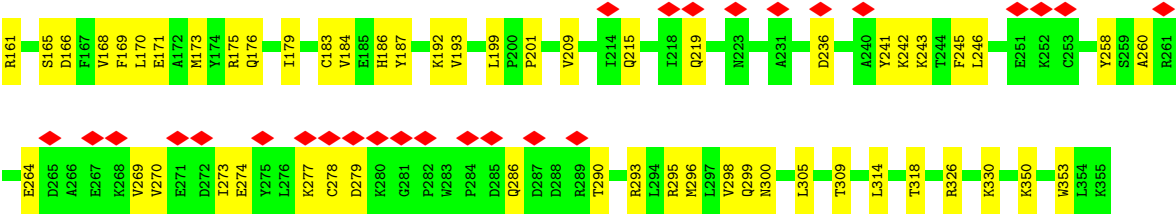


• Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



• Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63623	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.209	Depositor
Minimum map value	-0.092	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0222	Depositor
Map size ($\text{\AA}$)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UQ, SF4, PLX, CDL, FES, 2MR, ZN, 8Q1, PEE, ADP, MG, NDP, FMN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.17	0/3393	0.44	2/4584 (0.0%)
2	B	0.13	0/1443	0.33	0/1952
3	C	0.13	0/1279	0.34	0/1730
4	E	0.13	0/995	0.34	0/1340
5	F	0.16	0/702	0.41	0/945
6	G	0.19	0/673	0.49	0/911
6	X	0.14	0/705	0.37	0/956
7	H	0.13	0/929	0.33	0/1258
8	I	0.15	0/798	0.38	0/1079
9	J	0.16	0/2404	0.45	0/3245
10	K	0.09	0/365	0.29	0/493
11	L	0.09	0/1039	0.27	0/1403
12	M	0.14	0/5381	0.36	0/7291
13	N	0.17	0/1245	0.47	3/1694 (0.2%)
14	O	0.16	0/1699	0.46	3/2313 (0.1%)
15	P	0.12	0/1789	0.32	0/2436
16	Q	0.21	0/3451	0.49	6/4672 (0.1%)
17	S	0.12	0/582	0.30	0/783
18	T	0.10	0/755	0.28	0/1018
19	U	0.11	0/664	0.29	0/912
20	V	0.12	0/1042	0.29	0/1411
21	W	0.15	0/1198	0.31	0/1617
22	Y	0.14	0/626	0.33	0/857
23	Z	0.10	0/695	0.27	0/939
24	a	0.12	0/1195	0.33	0/1618
25	b	0.13	0/906	0.32	0/1232
26	c	0.16	0/1371	0.35	0/1875
27	d	0.13	0/1494	0.34	0/2015
28	e	0.13	0/916	0.39	0/1246
29	f	0.11	0/350	0.24	0/473
30	g	0.10	0/1031	0.27	0/1394
31	h	0.12	0/889	0.30	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.15	0/2773	0.37	1/3768 (0.0%)
33	j	0.16	0/819	0.39	0/1117
34	k	0.12	0/759	0.31	0/1029
35	l	0.17	0/4914	0.41	1/6683 (0.0%)
36	m	0.16	0/973	0.41	0/1320
37	n	0.21	0/468	0.62	1/633 (0.2%)
38	o	0.15	0/1092	0.35	0/1481
39	p	0.12	0/1590	0.33	0/2155
40	r	0.17	0/3723	0.43	2/5078 (0.0%)
41	s	0.19	0/2464	0.48	4/3369 (0.1%)
42	u	0.11	0/1436	0.31	0/1938
43	v	0.21	0/1016	0.55	1/1370 (0.1%)
44	w	0.14	0/2646	0.36	0/3584
All	All	0.15	0/66677	0.39	24/90407 (0.0%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	N	143	PRO	CA-N-CD	-8.87	99.58	112.00
16	Q	63	PRO	CA-C-N	8.61	125.95	119.66
16	Q	63	PRO	C-N-CA	8.61	125.95	119.66
41	s	86	TRP	N-CA-C	6.87	118.84	111.36
16	Q	217	VAL	N-CA-C	6.22	117.01	110.72
16	Q	224	ALA	N-CA-C	5.96	117.77	111.28
43	v	77	PHE	N-CA-C	5.71	117.50	111.28
13	N	141	SER	CA-C-N	5.70	129.35	120.68
13	N	141	SER	C-N-CA	5.70	129.35	120.68
37	n	16	LEU	N-CA-C	5.64	117.43	111.28
1	A	118	ASP	N-CA-C	5.57	117.35	111.28
41	s	93	TYR	CA-C-N	5.44	125.34	119.85
41	s	93	TYR	C-N-CA	5.44	125.34	119.85
1	A	136	HIS	N-CA-C	5.40	117.16	111.28
40	r	158	LEU	CA-C-N	5.37	125.01	119.05
40	r	158	LEU	C-N-CA	5.37	125.01	119.05
35	l	601	LEU	N-CA-C	5.30	117.14	111.36
14	O	225	CYS	N-CA-C	5.27	118.71	111.54
41	s	87	VAL	CB-CA-C	-5.23	108.80	114.35
14	O	226	GLU	CA-C-N	5.21	125.14	119.78
14	O	226	GLU	C-N-CA	5.21	125.14	119.78
32	i	89	MET	N-CA-C	5.04	116.78	111.28
16	Q	62	LYS	CA-C-N	5.02	125.55	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	62	LYS	C-N-CA	5.02	125.55	120.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3318	0	3280	110	0
2	B	1412	0	1363	40	0
3	C	1248	0	1254	34	0
4	E	971	0	975	23	0
5	F	691	0	704	16	0
6	G	664	0	613	22	0
6	X	693	0	664	26	0
7	H	910	0	950	14	0
8	I	780	0	808	10	0
9	J	2352	0	2396	65	0
10	K	355	0	329	19	0
11	L	1016	0	1016	21	0
12	M	5293	0	5324	117	0
13	N	1204	0	1162	23	0
14	O	1660	0	1659	53	0
15	P	1738	0	1693	23	0
16	Q	3377	0	3319	85	0
17	S	567	0	565	10	0
18	T	741	0	702	14	0
19	U	643	0	642	11	0
20	V	1021	0	1027	12	0
21	W	1167	0	1155	30	0
22	Y	600	0	539	16	0
23	Z	674	0	643	11	0
24	a	1161	0	1170	26	0
25	b	879	0	899	37	0
26	c	1315	0	1208	33	0
27	d	1461	0	1429	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	e	890	0	837	22	0
29	f	342	0	341	2	0
30	g	1000	0	994	15	0
31	h	867	0	871	18	0
32	i	2710	0	2874	98	0
33	j	800	0	855	31	0
34	k	748	0	799	22	0
35	l	4785	0	4933	153	0
36	m	951	0	962	40	0
37	n	456	0	433	19	0
38	o	1062	0	1072	16	0
39	p	1534	0	1470	36	0
40	r	3631	0	3839	136	0
41	s	2394	0	2508	86	0
42	u	1398	0	1378	20	0
43	v	992	0	908	40	0
44	w	2586	0	2542	88	0
45	A	8	0	0	2	0
45	B	16	0	0	0	0
45	C	8	0	0	1	0
45	M	16	0	0	0	0
46	A	31	0	19	5	0
47	B	51	0	82	6	0
47	U	51	0	82	6	0
47	i	47	0	71	18	0
47	j	47	0	71	18	0
47	l	92	0	138	38	0
47	m	41	0	59	23	0
47	r	51	0	82	5	0
48	C	52	0	88	4	0
48	a	52	0	88	11	0
48	g	52	0	88	5	0
48	j	52	0	88	4	0
48	r	104	0	176	7	0
49	G	35	0	0	0	0
49	X	35	0	0	2	0
50	J	48	0	23	8	0
51	M	4	0	0	0	0
51	O	4	0	0	0	0
52	M	1	0	0	0	0
53	N	51	0	46	13	0
53	a	91	0	132	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	g	100	0	156	7	0
53	i	66	0	76	13	0
53	l	199	0	307	20	0
53	n	78	0	103	20	0
54	T	1	0	0	0	0
55	s	28	0	31	7	0
56	w	27	0	11	13	0
All	All	66596	0	67121	1597	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1597) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:485:ASP:CB	12:M:680:LEU:HD13	1.62	1.30
50:J:401:NDP:O4D	50:J:401:NDP:C4D	1.68	1.22
1:A:287:THR:HG22	14:O:225:CYS:SG	1.80	1.21
1:A:129:GLU:OE2	1:A:287:THR:HG21	1.47	1.13
43:v:76:ASN:ND2	43:v:79:ALA:HB2	1.62	1.12
35:l:5:ALA:HB2	35:l:61:MET:SD	1.91	1.09
47:j:201:PEE:H70	41:s:53:LEU:HD23	1.10	1.08
1:A:119:GLU:HG2	1:A:127:ASP:HB2	1.36	1.08
32:i:91:ASN:HD22	32:i:92:PRO:HD2	1.09	1.08
32:i:11:MET:HE2	32:i:11:MET:HA	1.28	1.06
53:a:201:CDL:H532	47:l:704:PEE:H56	1.38	1.05
44:w:169:PHE:CD2	56:w:401:ADP:N1	2.25	1.04
53:n:101:CDL:H542	53:n:101:CDL:H581	1.42	1.02
35:l:590:SER:O	35:l:594:THR:HG22	1.58	1.01
1:A:119:GLU:CG	1:A:127:ASP:HB2	1.93	0.99
27:d:90:MET:HE3	40:r:47:GLU:OE1	1.58	0.99
27:d:90:MET:CE	40:r:47:GLU:OE1	2.11	0.99
37:n:13:VAL:CG1	40:r:14:MET:HG2	1.93	0.98
32:i:133:TRP:HE3	53:i:401:CDL:H391	1.25	0.98
44:w:165:SER:O	44:w:168:VAL:HG22	1.63	0.98
43:v:63:LEU:O	43:v:67:LEU:HD13	1.63	0.98
1:A:88:ARG:HG2	1:A:246:GLU:CD	1.89	0.97
16:Q:62:LYS:HG2	16:Q:63:PRO:HD2	1.46	0.97
1:A:287:THR:HG22	14:O:225:CYS:HG	1.16	0.96
44:w:169:PHE:CD2	56:w:401:ADP:C6	2.53	0.96
32:i:91:ASN:ND2	32:i:92:PRO:HD2	1.80	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:109:ASN:HD21	9:J:112:ASP:CG	1.76	0.94
14:O:200:ASP:OD2	14:O:219:ARG:HG3	1.67	0.94
47:j:201:PEE:C42	41:s:53:LEU:HD23	1.98	0.93
47:i:402:PEE:H37	47:i:402:PEE:H60	1.51	0.92
44:w:170:LEU:HD11	44:w:184:VAL:HG12	1.52	0.92
53:a:201:CDL:H251	53:a:201:CDL:H211	1.51	0.92
1:A:287:THR:CG2	14:O:225:CYS:SG	2.57	0.92
2:B:70:LEU:HD11	47:B:303:PEE:H65	1.49	0.91
3:C:50:LEU:HD13	47:j:201:PEE:H25	1.52	0.91
9:J:83:PRO:HA	9:J:106:MET:O	1.70	0.91
53:n:101:CDL:H271	53:n:101:CDL:H772	1.51	0.90
1:A:129:GLU:CD	1:A:287:THR:HG21	1.97	0.89
36:m:34:ILE:CG2	47:m:201:PEE:H44	2.03	0.89
44:w:168:VAL:HG11	44:w:241:TYR:HD1	1.38	0.89
32:i:133:TRP:CE3	53:i:401:CDL:H391	2.08	0.88
16:Q:182:ASN:HD22	16:Q:403:PRO:HB2	1.37	0.88
3:C:50:LEU:CD1	47:j:201:PEE:H25	2.02	0.88
3:C:50:LEU:HD13	47:j:201:PEE:C17	2.03	0.88
53:a:201:CDL:C53	47:l:704:PEE:H56	2.04	0.88
6:G:75:THR:O	6:G:77:GLU:N	2.07	0.87
1:A:129:GLU:OE2	1:A:287:THR:CG2	2.22	0.87
28:e:109:LEU:HD13	40:r:43:ASN:HB2	1.55	0.87
12:M:498:GLN:HB2	12:M:669:ASN:HD21	1.40	0.86
47:m:201:PEE:H25	47:m:201:PEE:C35	2.06	0.86
9:J:109:ASN:ND2	9:J:112:ASP:CG	2.33	0.86
32:i:268:GLN:HE22	32:i:272:LYS:HE3	1.40	0.85
25:b:104:ILE:HB	43:v:48:ASP:HB3	1.56	0.85
35:l:591:PHE:HA	35:l:594:THR:CG2	2.07	0.84
24:a:143:GLU:HG3	40:r:175:ASN:HD22	1.41	0.84
32:i:11:MET:HA	32:i:11:MET:CE	2.08	0.84
6:G:69:SER:N	16:Q:60:HIS:CE1	2.45	0.84
44:w:63:ASP:HB3	44:w:241:TYR:OH	1.79	0.83
44:w:169:PHE:CE2	56:w:401:ADP:C6	2.66	0.83
16:Q:62:LYS:CG	16:Q:63:PRO:HD2	2.09	0.83
37:n:13:VAL:HG12	40:r:14:MET:HG2	1.61	0.82
40:r:122:PHE:HE1	40:r:238:LEU:HB3	1.44	0.81
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.62	0.81
47:j:201:PEE:H59	47:j:201:PEE:H27	1.61	0.81
27:d:78:GLU:HB3	27:d:81:ASP:HB2	1.63	0.81
32:i:95:MET:HE2	32:i:149:ILE:N	1.96	0.81
32:i:11:MET:CE	53:i:401:CDL:H551	2.10	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:3:SER:O	53:N:201:CDL:HA22	1.81	0.80
44:w:242:LYS:HA	44:w:246:LEU:HD23	1.63	0.79
48:a:202:PLX:H282	48:a:202:PLX:C32	2.13	0.79
44:w:63:ASP:CB	44:w:241:TYR:OH	2.30	0.79
44:w:75:ARG:HB2	44:w:75:ARG:NH1	1.98	0.79
35:l:166:THR:CG2	47:l:703:PEE:H2	2.13	0.78
53:N:201:CDL:H711	41:s:43:TYR:OH	1.83	0.78
13:N:9:ARG:HD2	53:N:201:CDL:OB4	1.82	0.78
37:n:14:HIS:CE1	40:r:22:MET:HE2	2.19	0.78
41:s:233:MET:HE1	41:s:234:MET:HE2	1.66	0.78
36:m:34:ILE:HG22	47:m:201:PEE:H44	1.64	0.78
47:i:402:PEE:H28	47:i:402:PEE:C22	2.14	0.78
1:A:113:LEU:HD13	1:A:149:MET:HE1	1.66	0.77
44:w:168:VAL:HG11	44:w:241:TYR:CD1	2.20	0.77
35:l:591:PHE:O	35:l:594:THR:HG23	1.85	0.77
41:s:87:VAL:HG23	41:s:88:PRO:HD3	1.67	0.77
32:i:91:ASN:HD22	32:i:92:PRO:CD	1.95	0.77
32:i:95:MET:HE3	32:i:149:ILE:HG22	1.67	0.77
40:r:45:LEU:CD2	40:r:50:LEU:CD2	2.63	0.77
40:r:112:ALA:HB1	40:r:118:PHE:HB2	1.65	0.76
9:J:85:ARG:HD2	50:J:401:NDP:O1X	1.85	0.76
48:a:202:PLX:H282	48:a:202:PLX:H322	1.68	0.76
44:w:169:PHE:CG	56:w:401:ADP:N6	2.54	0.76
33:j:68:GLU:HG2	36:m:161:LEU:HD13	1.67	0.76
53:N:201:CDL:H541	53:N:201:CDL:H312	1.66	0.76
9:J:109:ASN:OD1	9:J:112:ASP:HB2	1.87	0.75
40:r:216:LEU:HG	40:r:220:HIS:CE1	2.22	0.75
16:Q:68:ASP:O	32:i:49:ASN:ND2	2.18	0.75
37:n:27:LEU:HD21	53:n:101:CDL:H112	1.69	0.75
7:H:7:LYS:HG3	7:H:8:THR:HG23	1.67	0.75
41:s:24:GLU:HG3	41:s:271:LEU:HD22	1.68	0.75
43:v:63:LEU:O	43:v:67:LEU:CD1	2.33	0.75
33:j:24:LEU:HD21	47:j:201:PEE:H63	1.67	0.75
47:m:201:PEE:H25	47:m:201:PEE:H56	1.67	0.75
28:e:109:LEU:CD1	40:r:43:ASN:HB2	2.17	0.74
35:l:5:ALA:CB	35:l:61:MET:SD	2.74	0.74
32:i:276:ILE:HG21	47:r:501:PEE:H14	1.66	0.74
35:l:4:PHE:HB2	35:l:53:MET:CE	2.17	0.74
12:M:472:PRO:O	12:M:510:TRP:NE1	2.17	0.74
39:p:44:MET:HA	39:p:47:ARG:HG2	1.68	0.74
9:J:106:MET:HE1	18:T:53:VAL:HG22	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:131:GLY:O	50:J:401:NDP:H51A	1.87	0.74
47:i:402:PEE:C25	47:i:402:PEE:H34	2.17	0.74
25:b:11:ARG:NH2	39:p:165:PRO:O	2.21	0.74
40:r:45:LEU:CD2	40:r:50:LEU:HD21	2.18	0.74
1:A:398:ARG:NH1	12:M:155:GLU:OE1	2.19	0.74
53:a:201:CDL:H251	53:a:201:CDL:C21	2.18	0.73
40:r:45:LEU:HD21	40:r:50:LEU:HD23	1.69	0.73
41:s:62:ARG:HH21	41:s:68:ILE:HB	1.53	0.73
6:G:69:SER:N	16:Q:60:HIS:HE1	1.87	0.73
35:l:589:LEU:O	35:l:593:ILE:HG13	1.89	0.72
3:C:196:ARG:HB2	9:J:85:ARG:NH1	2.03	0.72
53:a:201:CDL:H772	53:a:201:CDL:H201	1.71	0.72
26:c:110:ASP:OD1	40:r:278:ARG:NH2	2.22	0.72
37:n:27:LEU:HD21	53:n:101:CDL:C11	2.20	0.72
3:C:167:PRO:HG3	16:Q:222:MET:HE2	1.70	0.72
40:r:45:LEU:HD12	40:r:47:GLU:HB2	1.70	0.72
43:v:112:LYS:HD2	43:v:112:LYS:O	1.88	0.72
3:C:125:PRO:HB2	41:s:58:LYS:HE3	1.71	0.72
12:M:388:ASN:N	12:M:514:ASN:OD1	2.23	0.72
47:i:402:PEE:H28	47:i:402:PEE:H36	1.70	0.72
40:r:281:ASP:OD2	40:r:340:ARG:NH1	2.23	0.72
1:A:159:ARG:NH2	14:O:176:CYS:O	2.22	0.72
17:S:12:MET:HE2	41:s:23:VAL:HG21	1.70	0.71
32:i:11:MET:HE3	53:i:401:CDL:H551	1.72	0.71
20:V:42:ALA:HB2	35:l:593:ILE:HD11	1.73	0.71
44:w:114:LEU:HD21	56:w:401:ADP:H1'	1.72	0.71
32:i:267:ILE:HG12	32:i:279:PRO:HB3	1.71	0.71
16:Q:62:LYS:HG2	16:Q:63:PRO:CD	2.20	0.70
12:M:462:PHE:HA	12:M:465:ILE:HD12	1.72	0.70
32:i:95:MET:HE2	32:i:148:SER:C	2.17	0.70
12:M:128:CYS:SG	12:M:140:GLN:NE2	2.64	0.70
28:e:89:VAL:HG21	40:r:25:ILE:HG23	1.74	0.70
37:n:13:VAL:HG13	40:r:14:MET:HG2	1.73	0.70
25:b:99:GLU:HG2	35:l:61:MET:HE2	1.74	0.70
12:M:304:GLN:HG2	12:M:615:LEU:HD12	1.73	0.69
47:i:402:PEE:H34	47:i:402:PEE:H41	1.72	0.69
41:s:24:GLU:OE1	41:s:228:TYR:OH	2.09	0.69
1:A:174:ARG:HA	10:K:93:LEU:HD21	1.74	0.69
21:W:73:PRO:HA	42:u:44:MET:HE2	1.74	0.69
32:i:284:MET:O	47:i:402:PEE:H67	1.92	0.69
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:278:MET:O	32:i:282:MET:HG3	1.93	0.69
33:j:3:ILE:CD1	47:m:201:PEE:H50	2.22	0.69
40:r:122:PHE:CZ	40:r:206:LYS:HD3	2.27	0.69
9:J:95:ARG:HB2	9:J:96:PRO:HD3	1.74	0.69
5:F:40:ARG:HH22	5:F:84:ALA:HB1	1.58	0.68
53:l:701:CDL:H391	40:r:371:PRO:HD2	1.75	0.68
41:s:195:ARG:HD3	41:s:231:ILE:HD11	1.73	0.68
41:s:18:ALA:HB2	55:s:401:UQ:H152	1.76	0.68
41:s:146:LEU:HD11	41:s:192:GLU:HG3	1.74	0.68
3:C:196:ARG:HB2	9:J:85:ARG:HH11	1.57	0.68
13:N:120:THR:HG22	13:N:122:GLN:H	1.57	0.68
43:v:110:GLN:HA	43:v:110:GLN:OE1	1.92	0.68
1:A:296:LEU:HD13	1:A:335:VAL:HG13	1.76	0.68
1:A:132:ARG:HB3	1:A:165:GLU:CB	2.24	0.67
1:A:217:GLU:OE1	11:L:171:ARG:NH2	2.27	0.67
35:l:419:THR:HA	35:l:422:TYR:CE2	2.30	0.67
26:c:117:VAL:HG21	35:l:539:TYR:HB2	1.76	0.67
32:i:108:LEU:HD11	32:i:191:THR:HG21	1.76	0.67
33:j:4:MET:HE3	47:m:201:PEE:H21	1.77	0.67
1:A:41:ILE:O	1:A:137:LYS:NZ	2.27	0.67
44:w:88:GLU:OE2	44:w:161:ARG:NH1	2.28	0.67
6:X:103:HIS:HE1	6:X:139:MET:HE3	1.60	0.67
48:a:202:PLX:H101	40:r:40:SER:HB3	1.76	0.67
1:A:88:ARG:HG2	1:A:246:GLU:OE1	1.95	0.66
12:M:197:THR:N	14:O:114:GLU:OE2	2.28	0.66
12:M:677:GLN:OE1	12:M:677:GLN:N	2.27	0.66
36:m:41:CYS:SG	36:m:57:PHE:HB2	2.36	0.66
2:B:76:TYR:HE2	41:s:33:LEU:HB2	1.60	0.66
14:O:182:ASN:ND2	14:O:194:GLU:OE2	2.28	0.66
14:O:88:ARG:NH2	14:O:190:ASP:OD2	2.28	0.66
44:w:176:GLN:NE2	44:w:236:ASP:OD2	2.28	0.66
1:A:263:ALA:HA	1:A:271:SER:HB2	1.77	0.66
6:X:103:HIS:CE1	6:X:139:MET:HE3	2.31	0.66
35:l:3:PRO:HG2	35:l:53:MET:HE1	1.77	0.66
1:A:398:ARG:NH2	1:A:408:GLU:OE1	2.29	0.66
25:b:81:ILE:HG23	47:l:704:PEE:H58	1.78	0.66
26:c:116:ARG:HG2	47:l:703:PEE:H49	1.77	0.66
37:n:14:HIS:CE1	40:r:26:ASN:OD1	2.49	0.66
6:X:123:GLU:HG2	6:X:129:GLU:HA	1.79	0.65
34:k:22:TYR:O	35:l:585:LYS:NZ	2.24	0.65
35:l:55:MET:HE2	35:l:471:ASN:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:o:80:PHE:HE1	38:o:86:THR:HG21	1.60	0.65
53:g:202:CDL:H852	53:n:101:CDL:C82	2.26	0.65
1:A:46:TYR:O	14:O:224:SER:CB	2.45	0.65
12:M:445:LEU:HG	12:M:460:HIS:HE1	1.62	0.65
12:M:478:SER:O	12:M:482:GLN:HG2	1.97	0.65
25:b:105:PHE:HB2	43:v:68:LYS:HD3	1.77	0.65
40:r:45:LEU:CD2	40:r:50:LEU:HD23	2.25	0.65
40:r:447:LEU:HD11	48:r:503:PLX:H371	1.79	0.65
36:m:11:THR:O	36:m:15:ILE:HG12	1.97	0.64
1:A:50:ASP:O	1:A:59:ARG:NH2	2.30	0.64
40:r:225:ILE:HD13	40:r:331:ASN:HB2	1.78	0.64
41:s:95:LEU:HD23	41:s:95:LEU:O	1.96	0.64
22:Y:87:PRO:HB2	22:Y:92:TRP:HZ2	1.62	0.64
33:j:60:ILE:HG21	36:m:168:ILE:HG21	1.79	0.64
53:n:101:CDL:H161	53:n:101:CDL:HB31	1.78	0.64
38:o:46:GLU:OE1	38:o:50:GLN:NE2	2.31	0.64
1:A:79:GLU:OE2	1:A:259:GLY:N	2.29	0.64
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.31	0.64
47:i:402:PEE:H36	47:i:402:PEE:C18	2.27	0.64
35:l:558:LEU:HB3	40:r:214:LEU:HD21	1.79	0.64
36:m:34:ILE:HG22	47:m:201:PEE:C26	2.26	0.64
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.31	0.64
1:A:60:GLY:O	1:A:256:ARG:NH1	2.31	0.64
13:N:143:PRO:HD2	13:N:143:PRO:O	1.98	0.64
47:j:201:PEE:H27	47:j:201:PEE:C36	2.28	0.64
1:A:104:LYS:HG2	1:A:105:PRO:HD2	1.79	0.64
47:m:201:PEE:O4	47:m:201:PEE:H7	1.92	0.64
40:r:216:LEU:HG	40:r:220:HIS:HE1	1.62	0.64
3:C:50:LEU:HD13	47:j:201:PEE:H26	1.79	0.64
11:L:105:GLU:HA	12:M:611:THR:HG21	1.80	0.64
26:c:128:THR:O	26:c:132:HIS:HD2	1.80	0.64
24:a:127:ASP:OD1	48:a:202:PLX:H12	1.97	0.63
2:B:94:SER:OG	16:Q:215:GLU:OE2	2.16	0.63
10:K:100:GLN:HB3	14:O:71:PRO:HA	1.81	0.63
12:M:389:THR:HB	12:M:473:MET:HE3	1.80	0.63
27:d:144:SER:O	27:d:158:LYS:NZ	2.26	0.63
47:U:101:PEE:H34	41:s:302:MET:HE1	1.79	0.63
28:e:109:LEU:HD13	40:r:43:ASN:CB	2.26	0.63
53:g:202:CDL:H361	32:i:246:VAL:HG21	1.79	0.63
40:r:403:THR:HA	40:r:406:TYR:CE2	2.34	0.63
41:s:26:LYS:HD2	41:s:36:GLY:HA3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:95:LEU:HD22	41:s:96:ILE:HG13	1.81	0.63
9:J:206:ILE:N	50:J:401:NDP:H71N	1.97	0.63
16:Q:65:PRO:HB2	16:Q:67:ASN:O	1.98	0.63
33:j:24:LEU:HD21	47:j:201:PEE:C38	2.27	0.63
41:s:95:LEU:HD23	41:s:95:LEU:C	2.23	0.63
1:A:119:GLU:HA	1:A:119:GLU:OE2	1.99	0.63
12:M:193:ASP:OD1	14:O:111:ARG:NH2	2.29	0.63
43:v:76:ASN:CG	43:v:79:ALA:HB2	2.23	0.63
44:w:129:TYR:OH	44:w:186:HIS:ND1	2.26	0.63
3:C:126:GLU:O	9:J:89:TYR:OH	2.17	0.63
26:c:33:THR:OG1	26:c:35:ASP:OD1	2.17	0.63
33:j:64:LEU:HD13	36:m:165:VAL:HG22	1.80	0.63
35:l:72:GLN:NE2	40:r:459:TYR:O	2.32	0.63
2:B:192:ASN:ND2	18:T:61:GLU:OE2	2.32	0.62
9:J:369:VAL:HG12	9:J:370:LYS:HG2	1.81	0.62
12:M:483:ARG:HH21	12:M:483:ARG:HB3	1.64	0.62
40:r:198:ALA:HB2	47:r:501:PEE:H30	1.81	0.62
14:O:179:ALA:HB3	14:O:185:MET:HG2	1.80	0.62
24:a:152:LYS:HD3	30:g:96:VAL:HG21	1.80	0.62
25:b:105:PHE:CB	43:v:68:LYS:HD3	2.28	0.62
47:j:201:PEE:H70	41:s:53:LEU:CD2	2.06	0.62
35:l:66:TRP:CG	47:l:704:PEE:H19	2.34	0.62
15:P:44:ARG:HE	15:P:45:PRO:HD3	1.64	0.62
19:U:23:PHE:CD2	47:U:101:PEE:H58	2.35	0.62
12:M:244:GLU:OE1	12:M:266:ARG:NH1	2.31	0.62
25:b:123:PHE:HB3	43:v:40:VAL:HG11	1.79	0.62
53:n:101:CDL:H122	53:n:101:CDL:H272	1.80	0.62
44:w:76:GLU:OE1	44:w:76:GLU:HA	1.99	0.62
35:l:4:PHE:HB2	35:l:53:MET:HE2	1.81	0.62
40:r:198:ALA:HB2	47:r:501:PEE:H22	1.81	0.62
41:s:102:VAL:HG21	41:s:154:LEU:HD11	1.81	0.62
36:m:30:GLY:O	36:m:34:ILE:HD12	2.00	0.62
44:w:170:LEU:CD1	44:w:184:VAL:HG12	2.27	0.62
12:M:624:ARG:NH2	12:M:637:ASP:OD1	2.29	0.62
30:g:56:VAL:HG21	40:r:17:MET:HE1	1.82	0.62
40:r:122:PHE:CE1	40:r:238:LEU:HB3	2.31	0.62
38:o:59:VAL:HG23	40:r:423:ILE:HG12	1.82	0.61
41:s:20:LEU:HD12	41:s:20:LEU:O	2.00	0.61
41:s:62:ARG:HD3	41:s:64:ALA:H	1.65	0.61
16:Q:133:LEU:CD2	16:Q:228:ARG:HD3	2.30	0.61
32:i:316:GLN:NE2	44:w:95:ASP:OD1	2.28	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:83:PRO:HB2	9:J:108:TRP:CD1	2.36	0.61
21:W:57:ARG:HB3	41:s:316:PRO:HG3	1.83	0.61
37:n:14:HIS:HE1	40:r:22:MET:HE2	1.65	0.61
24:a:97:GLU:OE1	27:d:60:ARG:NH1	2.33	0.61
24:a:134:GLU:OE1	37:n:57:TRP:NE1	2.27	0.61
53:a:201:CDL:OA7	53:a:201:CDL:HA61	2.00	0.61
32:i:42:PRO:HG3	36:m:167:VAL:HG13	1.81	0.61
1:A:116:ASN:ND2	1:A:207:GLY:O	2.32	0.61
12:M:460:HIS:HD2	12:M:461:PRO:HD2	1.65	0.61
23:Z:22:TRP:HB3	23:Z:50:ALA:HB3	1.83	0.61
25:b:12:LEU:O	25:b:16:ARG:HG3	2.01	0.61
32:i:280:THR:O	32:i:284:MET:HG2	2.01	0.61
40:r:42:LEU:HG	40:r:67:VAL:HG21	1.82	0.61
12:M:133:GLN:HG3	12:M:136:GLU:HG3	1.81	0.61
6:G:119:ILE:HD13	6:G:135:ALA:HB1	1.82	0.61
7:H:77:ILE:O	7:H:81:ILE:HD12	2.00	0.61
53:a:201:CDL:H521	47:l:704:PEE:H13	1.82	0.61
19:U:27:GLY:O	19:U:31:ILE:HG13	2.01	0.61
21:W:90:ASN:ND2	21:W:123:GLU:O	2.34	0.61
32:i:133:TRP:HE3	53:i:401:CDL:C39	2.07	0.61
32:i:77:ASN:OD1	32:i:89:MET:O	2.18	0.60
32:i:236:LYS:HG2	32:i:237:MET:HG3	1.82	0.60
53:n:101:CDL:H1	53:n:101:CDL:H151	1.83	0.60
7:H:44:TYR:HB2	15:P:68:ILE:HG23	1.81	0.60
9:J:209:ARG:NH2	9:J:351:GLU:OE2	2.34	0.60
12:M:638:THR:OG1	12:M:640:ASP:OD1	2.18	0.60
34:k:80:MET:HE2	36:m:172:THR:HA	1.82	0.60
28:e:102:GLY:HA3	40:r:39:LEU:CD2	2.31	0.60
32:i:128:LEU:HD12	32:i:216:PHE:HB3	1.84	0.60
53:i:401:CDL:HB31	44:w:40:PRO:HB2	1.83	0.60
41:s:281:ARG:HB2	41:s:284:GLN:HG3	1.82	0.60
6:G:75:THR:O	6:G:76:LEU:C	2.44	0.60
33:j:3:ILE:HD13	47:m:201:PEE:C32	2.31	0.60
35:l:161:ARG:NH2	39:p:88:GLY:O	2.33	0.60
35:l:391:SER:O	35:l:395:ILE:HG12	2.01	0.60
53:l:701:CDL:H401	40:r:445:LEU:HD22	1.83	0.60
14:O:134:VAL:HG12	14:O:186:VAL:HG12	1.82	0.60
15:P:125:ARG:NH2	15:P:201:ASP:OD2	2.27	0.60
53:a:201:CDL:H752	28:e:103:SER:HB3	1.83	0.60
39:p:29:SER:HB3	39:p:76:HIS:HD2	1.67	0.60
43:v:60:ALA:O	43:v:64:ILE:HG13	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:177:THR:HG21	2:B:182:GLU:HB2	1.84	0.60
9:J:102:GLN:OE1	9:J:102:GLN:HA	1.99	0.60
12:M:388:ASN:ND2	12:M:513:MET:O	2.25	0.60
26:c:38:PRO:HB2	38:o:75:ASN:HD22	1.67	0.60
2:B:70:LEU:CD1	47:B:303:PEE:H65	2.26	0.60
3:C:50:LEU:HD11	47:j:201:PEE:H25	1.84	0.60
12:M:63:PHE:O	12:M:181:ARG:NH2	2.35	0.60
12:M:650:SER:OG	12:M:652:ASN:OD1	2.19	0.60
14:O:191:ASN:C	14:O:191:ASN:HD22	2.06	0.60
1:A:369:ARG:NH2	14:O:136:THR:OG1	2.33	0.60
53:a:201:CDL:H761	53:a:201:CDL:C19	2.31	0.60
43:v:112:LYS:HD2	43:v:112:LYS:C	2.27	0.60
44:w:169:PHE:CD1	56:w:401:ADP:N6	2.70	0.60
10:K:95:LYS:HE2	10:K:96:PHE:HE1	1.67	0.59
35:l:245:ALA:O	35:l:249:SER:OG	2.20	0.59
4:E:37:ARG:HH22	6:G:132:ASP:HB2	1.67	0.59
11:L:109:ASN:ND2	11:L:111:LEU:O	2.35	0.59
4:E:47:VAL:HA	4:E:52:LEU:HD13	1.84	0.59
25:b:73:THR:HA	25:b:77:ILE:HD12	1.84	0.59
36:m:34:ILE:CG2	47:m:201:PEE:C26	2.78	0.59
42:u:121:ASP:OD1	42:u:122:LEU:N	2.35	0.59
28:e:58:ASP:OD2	44:w:326:ARG:NE	2.33	0.59
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.84	0.59
41:s:200:LEU:HD11	41:s:285:LEU:HD21	1.84	0.59
7:H:116:ILE:HG21	11:L:96:LYS:HE3	1.83	0.59
12:M:463:SER:O	12:M:467:LYS:HG2	2.03	0.59
12:M:485:ASP:CB	12:M:680:LEU:CD1	2.58	0.59
32:i:190:MET:HE2	32:i:205:LEU:HA	1.83	0.59
32:i:268:GLN:NE2	32:i:272:LYS:HE3	2.16	0.59
53:a:201:CDL:H201	53:a:201:CDL:C76	2.33	0.59
9:J:108:TRP:CE3	9:J:116:ILE:HG12	2.37	0.58
14:O:84:ASP:O	14:O:88:ARG:HG3	2.03	0.58
25:b:81:ILE:HG23	47:l:704:PEE:C36	2.33	0.58
25:b:100:ARG:HB3	35:l:60:GLU:HB2	1.85	0.58
27:d:36:ILE:O	27:d:40:LEU:HD23	2.03	0.58
35:l:145:GLU:OE1	35:l:176:ARG:NH1	2.36	0.58
25:b:89:HIS:CD2	47:l:704:PEE:H49	2.39	0.58
53:n:101:CDL:H542	53:n:101:CDL:C58	2.23	0.58
33:j:3:ILE:HD13	47:m:201:PEE:H50	1.85	0.58
33:j:3:ILE:CG2	47:m:201:PEE:H13	2.32	0.58
33:j:29:ALA:O	47:j:201:PEE:H12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:l:704:PEE:O1P	47:l:704:PEE:H8	2.03	0.58
4:E:62:LYS:O	4:E:66:MET:HG2	2.03	0.58
53:a:201:CDL:H322	47:l:704:PEE:H62	1.84	0.58
22:Y:72:ARG:NH1	22:Y:76:ASP:OD2	2.36	0.58
41:s:55:LEU:HD13	41:s:221:ALA:HB2	1.86	0.58
44:w:274:GLU:O	44:w:277:LYS:NZ	2.36	0.58
1:A:267:ARG:HH22	1:A:341:ALA:HB2	1.67	0.58
35:l:286:LEU:HD22	35:l:411:MET:SD	2.43	0.58
2:B:96:ARG:O	16:Q:219:GLY:HA3	2.04	0.58
40:r:126:LEU:HD12	40:r:149:PHE:CZ	2.39	0.58
2:B:68:ARG:NH1	16:Q:260:GLU:OE2	2.28	0.58
5:F:55:ILE:HD13	12:M:381:LEU:HD23	1.84	0.58
29:f:47:THR:HG23	30:g:65:LEU:HD22	1.85	0.58
33:j:18:VAL:HG22	41:s:222:MET:HG3	1.86	0.58
34:k:8:ILE:HG21	34:k:43:MET:HB2	1.85	0.58
40:r:45:LEU:HD23	40:r:45:LEU:H	1.68	0.58
21:W:5:LYS:HD2	21:W:6:VAL:H	1.68	0.58
26:c:58:ARG:NE	26:c:60:GLU:OE2	2.36	0.58
53:a:201:CDL:H201	53:a:201:CDL:C77	2.33	0.58
26:c:133:LEU:HD22	26:c:133:LEU:O	2.04	0.58
3:C:184:ILE:O	3:C:187:GLU:HG2	2.03	0.57
21:W:89:GLU:O	21:W:93:GLU:HG2	2.04	0.57
53:i:401:CDL:H171	53:i:401:CDL:H132	1.85	0.57
41:s:87:VAL:HG12	41:s:95:LEU:HD13	1.85	0.57
33:j:73:LEU:O	41:s:160:TYR:OH	2.21	0.57
35:l:142:ILE:HG12	40:r:370:PRO:HB2	1.84	0.57
5:F:58:CYS:HB2	5:F:61:VAL:HB	1.85	0.57
25:b:74:HIS:NE2	35:l:35:TYR:OH	2.26	0.57
1:A:177:TYR:OH	1:A:194:ASP:OD1	2.22	0.57
40:r:225:ILE:O	40:r:229:MET:HG3	2.04	0.57
41:s:13:ILE:O	41:s:17:VAL:HG22	2.03	0.57
15:P:187:ILE:HG23	15:P:188:LEU:HG	1.86	0.57
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.39	0.57
40:r:237:LYS:HD2	40:r:316:MET:HB3	1.86	0.57
44:w:63:ASP:HB2	44:w:241:TYR:OH	2.04	0.57
22:Y:69:ILE:HD13	35:l:383:MET:HE2	1.86	0.57
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.39	0.57
36:m:57:PHE:CZ	41:s:111:LEU:HD11	2.39	0.57
31:h:18:MET:HE1	36:m:153:LEU:HD11	1.86	0.57
9:J:104:ILE:N	9:J:104:ILE:HD12	2.20	0.57
1:A:119:GLU:CD	1:A:127:ASP:HB2	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:THR:O	2:B:187:LYS:NZ	2.38	0.57
6:G:75:THR:C	6:G:77:GLU:N	2.60	0.57
21:W:30:LEU:HB3	21:W:35:MET:HE3	1.86	0.57
6:X:155:TYR:CE1	25:b:23:LEU:HB3	2.39	0.57
2:B:177:THR:HG22	2:B:179:THR:H	1.68	0.57
5:F:41:TYR:CE2	5:F:55:ILE:HD11	2.40	0.57
9:J:79:GLN:HG3	9:J:102:GLN:O	2.04	0.57
53:a:201:CDL:OB7	53:a:201:CDL:HB61	2.03	0.57
25:b:19:ARG:HE	39:p:173:ARG:HH21	1.51	0.56
32:i:96:THR:O	32:i:100:MET:HG3	2.05	0.56
53:i:401:CDL:OB4	44:w:40:PRO:HG3	2.04	0.56
35:l:161:ARG:HA	39:p:92:GLU:HB2	1.87	0.56
5:F:24:CYS:N	5:F:58:CYS:SG	2.79	0.56
16:Q:46:GLN:HB3	47:i:402:PEE:H6	1.70	0.56
16:Q:156:GLU:HG3	16:Q:229:PRO:O	2.06	0.56
6:X:93:ILE:HD11	6:X:110:LEU:HD11	1.86	0.56
26:c:156:VAL:HG12	43:v:99:MET:HG2	1.87	0.56
37:n:50:ARG:HB2	37:n:53:GLU:HB2	1.86	0.56
2:B:99:GLY:CA	2:B:170:GLY:O	2.53	0.56
41:s:87:VAL:CG2	41:s:88:PRO:HD3	2.36	0.56
44:w:165:SER:O	44:w:168:VAL:CG2	2.47	0.56
25:b:25:ASP:OD2	39:p:125:TRP:NE1	2.32	0.56
32:i:88:LYS:NZ	32:i:147:GLN:O	2.39	0.56
35:l:66:TRP:CZ3	47:l:704:PEE:H32	2.40	0.56
12:M:373:PRO:HD2	12:M:481:LEU:HD13	1.87	0.56
12:M:399:VAL:HG21	12:M:466:LEU:HG	1.87	0.56
38:o:23:TYR:OH	39:p:68:GLU:OE1	2.24	0.56
39:p:35:ASP:OD1	39:p:36:LYS:N	2.38	0.56
43:v:76:ASN:ND2	43:v:79:ALA:CB	2.54	0.56
22:Y:94:ASP:HB3	22:Y:99:ILE:HB	1.87	0.56
27:d:163:MET:HG3	28:e:149:LEU:HD11	1.88	0.56
32:i:95:MET:CE	32:i:149:ILE:HG22	2.34	0.56
33:j:17:LEU:HA	33:j:20:ILE:HG12	1.87	0.56
33:j:79:SER:HA	33:j:87:MET:HE2	1.88	0.56
44:w:215:GLN:O	44:w:219:GLN:HG2	2.04	0.56
25:b:121:LYS:HD3	43:v:40:VAL:HA	1.88	0.56
40:r:312:ALA:O	40:r:316:MET:HG3	2.06	0.56
43:v:76:ASN:HD21	43:v:79:ALA:HB2	1.60	0.56
47:B:303:PEE:H64	41:s:273:ILE:HD11	1.88	0.56
20:V:69:ILE:HG13	20:V:100:THR:HG21	1.88	0.56
26:c:153:TYR:HB3	35:l:403:TYR:HD1	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:389:THR:CB	12:M:514:ASN:HD21	2.19	0.55
12:M:483:ARG:HB3	12:M:483:ARG:NH2	2.20	0.55
32:i:325:LEU:HD13	53:i:401:CDL:H132	1.88	0.55
35:l:363:TYR:HA	35:l:370:THR:HG21	1.88	0.55
35:l:591:PHE:O	35:l:595:ILE:HG13	2.06	0.55
3:C:59:ARG:NH1	48:C:302:PLX:O3	2.39	0.55
39:p:132:SER:O	39:p:136:GLU:HG3	2.05	0.55
41:s:69:SER:O	41:s:73:ILE:HG12	2.06	0.55
44:w:139:ARG:NH1	44:w:166:ASP:OD2	2.39	0.55
3:C:85:ASP:O	3:C:88:ARG:HG2	2.06	0.55
7:H:76:GLN:O	7:H:79:GLU:HG2	2.06	0.55
40:r:45:LEU:HD22	40:r:50:LEU:HD21	1.89	0.55
42:u:9:THR:OG1	42:u:12:ASP:OD1	2.24	0.55
1:A:119:GLU:HG2	1:A:127:ASP:CB	2.22	0.55
1:A:152:ARG:NH2	10:K:99:PRO:O	2.40	0.55
11:L:165:SER:O	11:L:171:ARG:NH1	2.38	0.55
25:b:100:ARG:HD3	35:l:60:GLU:HG3	1.87	0.55
32:i:314:LYS:NZ	44:w:309:THR:OG1	2.36	0.55
44:w:170:LEU:HD12	44:w:179:ILE:HD11	1.87	0.55
9:J:81:ILE:HD12	9:J:81:ILE:N	2.22	0.55
35:l:591:PHE:CA	35:l:594:THR:CG2	2.83	0.55
36:m:17:PHE:HA	36:m:20:PHE:CE2	2.42	0.55
2:B:184:LEU:HD23	11:L:112:MET:HG3	1.89	0.55
24:a:139:ILE:HG23	40:r:54:LEU:HD23	1.87	0.55
53:a:201:CDL:H391	53:a:201:CDL:H432	1.87	0.55
25:b:86:LEU:HA	25:b:90:VAL:HB	1.88	0.55
27:d:86:PHE:O	27:d:90:MET:HG2	2.07	0.55
35:l:591:PHE:HA	35:l:594:THR:HG22	1.89	0.55
9:J:157:LYS:NZ	9:J:197:GLU:OE1	2.38	0.55
16:Q:46:GLN:HB3	47:i:402:PEE:N	2.22	0.55
16:Q:357:LYS:HD3	16:Q:364:SER:HB3	1.87	0.55
6:X:114:ASP:O	6:X:118:ILE:HG12	2.07	0.55
53:l:702:CDL:H741	53:l:702:CDL:H532	1.88	0.55
53:n:101:CDL:H272	53:n:101:CDL:C12	2.37	0.55
43:v:103:GLU:O	43:v:107:ARG:HG2	2.07	0.55
1:A:269:ARG:NH1	1:A:269:ARG:HB2	2.22	0.55
1:A:380:GLY:O	1:A:386:ARG:NH1	2.39	0.55
6:G:118:ILE:O	6:G:122:MET:HG2	2.07	0.55
11:L:90:GLY:HA3	15:P:238:PRO:HB2	1.88	0.55
35:l:359:MET:O	35:l:436:ARG:NH2	2.39	0.55
35:l:561:ILE:HG22	35:l:562:LEU:HD12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ARG:HH22	10:K:77:GLN:HG2	1.71	0.55
1:A:385:CYS:HB3	45:A:501:SF4:S2	2.46	0.55
2:B:85:ASN:OD1	3:C:88:ARG:NH2	2.40	0.55
9:J:238:GLN:NE2	9:J:269:ASN:O	2.39	0.55
37:n:14:HIS:CE1	40:r:22:MET:CE	2.87	0.55
12:M:370:GLU:CG	12:M:482:GLN:HE22	2.19	0.54
35:l:83:ASP:OD2	35:l:262:ARG:NH1	2.39	0.54
35:l:152:PHE:HB2	35:l:172:ILE:HD11	1.90	0.54
40:r:158:LEU:N	40:r:159:PRO:CD	2.70	0.54
40:r:299:VAL:O	40:r:303:ILE:HG12	2.07	0.54
41:s:87:VAL:N	41:s:88:PRO:HD2	2.22	0.54
43:v:19:PRO:HA	43:v:22:MET:HE3	1.90	0.54
44:w:241:TYR:O	44:w:245:PHE:HB3	2.08	0.54
1:A:132:ARG:HB3	1:A:165:GLU:HB2	1.88	0.54
9:J:88:PRO:O	9:J:91:THR:HG22	2.08	0.54
14:O:110:MET:O	14:O:114:GLU:HG3	2.07	0.54
16:Q:216:ARG:NH1	16:Q:243:ASP:OD2	2.23	0.54
39:p:25:ARG:NH1	39:p:28:GLU:OE2	2.39	0.54
5:F:39:LYS:HB3	5:F:40:ARG:HD3	1.88	0.54
40:r:373:ILE:HD11	40:r:444:LEU:HD23	1.88	0.54
9:J:133:GLU:OE2	9:J:318:LYS:NZ	2.36	0.54
10:K:91:VAL:O	10:K:94:SER:OG	2.25	0.54
12:M:476:LEU:HD21	12:M:481:LEU:HD21	1.89	0.54
20:V:121:THR:O	20:V:125:VAL:HG23	2.07	0.54
6:X:105:MET:HG3	6:X:110:LEU:O	2.06	0.54
53:g:202:CDL:H441	40:r:101:LEU:HD13	1.89	0.54
32:i:95:MET:HE2	32:i:149:ILE:CA	2.36	0.54
32:i:325:LEU:HD12	53:i:401:CDL:H121	1.89	0.54
35:l:227:PHE:O	35:l:230:HIS:ND1	2.38	0.54
35:l:366:MET:HB2	35:l:445:GLU:OE1	2.08	0.54
4:E:57:LYS:NZ	4:E:61:ASP:OD2	2.40	0.54
13:N:140:PRO:HB2	13:N:142:THR:HG22	1.90	0.54
14:O:130:TYR:HA	14:O:189:ASN:HD21	1.72	0.54
16:Q:184:ILE:HD11	16:Q:251:PHE:CZ	2.43	0.54
44:w:143:TYR:OH	44:w:199:LEU:O	2.20	0.54
9:J:89:TYR:C	9:J:89:TYR:CD1	2.85	0.54
16:Q:446:ASP:OD1	41:s:281:ARG:NH1	2.40	0.54
30:g:12:PRO:HB3	31:h:5:ASP:HB3	1.90	0.54
31:h:69:ARG:O	31:h:73:MET:HG3	2.07	0.54
35:l:452:ASN:HA	35:l:455:LYS:HG2	1.90	0.54
44:w:63:ASP:CB	44:w:241:TYR:HH	2.18	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:2:PRO:O	27:d:7:LYS:NZ	2.41	0.54
35:l:172:ILE:O	35:l:176:ARG:HG2	2.08	0.54
6:G:120:MET:HA	6:G:123:GLU:OE1	2.08	0.54
9:J:212:ARG:HH22	50:J:401:NDP:PA	2.31	0.54
12:M:394:VAL:HG22	12:M:473:MET:HE1	1.89	0.54
14:O:169:PHE:HE2	14:O:205:ILE:HG23	1.73	0.54
16:Q:136:PHE:HB3	16:Q:147:ASN:HB3	1.90	0.54
53:g:202:CDL:H742	53:g:202:CDL:H271	1.90	0.54
31:h:18:MET:HG2	32:i:25:HIS:HE2	1.72	0.54
1:A:138:LEU:HD13	1:A:245:VAL:HG13	1.89	0.54
4:E:98:LYS:HB3	4:E:102:HIS:HB2	1.90	0.54
12:M:680:LEU:HD12	12:M:680:LEU:N	2.23	0.54
16:Q:204:PHE:HA	16:Q:207:ARG:HB2	1.90	0.54
35:l:591:PHE:HA	35:l:594:THR:HG21	1.89	0.54
41:s:170:GLU:OE1	42:u:98:ARG:NH1	2.41	0.54
42:u:137:LEU:HD12	42:u:138:PRO:HD2	1.90	0.54
44:w:72:ARG:NH2	44:w:264:GLU:OE1	2.41	0.54
3:C:188:LYS:HD3	3:C:191:ARG:HE	1.73	0.54
11:L:78:ARG:NH2	12:M:249:GLU:OE2	2.35	0.54
53:N:201:CDL:C55	53:N:201:CDL:C32	2.85	0.54
22:Y:73:PHE:HA	35:l:385:TYR:HE2	1.72	0.54
27:d:142:ARG:NE	28:e:138:GLU:O	2.38	0.54
40:r:231:LEU:HD23	40:r:235:LEU:HD12	1.90	0.54
1:A:125:CYS:H	1:A:277:ASN:HD22	1.56	0.53
2:B:99:GLY:N	2:B:170:GLY:O	2.42	0.53
4:E:15:THR:OG1	11:L:55:VAL:O	2.24	0.53
53:i:401:CDL:HB31	44:w:40:PRO:CB	2.37	0.53
35:l:298:ILE:O	35:l:302:VAL:HG23	2.09	0.53
44:w:168:VAL:CG1	44:w:241:TYR:HA	2.39	0.53
2:B:211:TYR:CZ	8:I:39:PRO:HG3	2.43	0.53
7:H:35:LEU:HD13	7:H:49:GLU:HG2	1.90	0.53
53:N:201:CDL:CA7	53:N:201:CDL:C34	2.86	0.53
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.33	0.53
27:d:119:GLU:HG2	43:v:52:MET:HA	1.90	0.53
2:B:99:GLY:O	2:B:169:GLU:HG2	2.09	0.53
4:E:114:ARG:HD3	4:E:115:PRO:HD2	1.90	0.53
44:w:171:GLU:O	44:w:175:ARG:HG3	2.09	0.53
7:H:7:LYS:HD3	7:H:8:THR:H	1.73	0.53
4:E:56:VAL:HG12	4:E:60:ARG:HD2	1.91	0.53
53:i:401:CDL:OA7	53:i:401:CDL:HA62	2.07	0.53
40:r:196:TRP:CD1	40:r:250:LEU:HB3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:39:TRP:O	4:E:43:VAL:HG23	2.09	0.53
13:N:3:LEU:HD11	53:N:201:CDL:H311	1.91	0.53
32:i:320:THR:HG21	44:w:300:ASN:HA	1.91	0.53
47:m:201:PEE:H25	47:m:201:PEE:H57	1.89	0.53
41:s:24:GLU:OE2	41:s:274:ARG:NH1	2.42	0.53
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	1.91	0.53
47:i:402:PEE:H34	47:i:402:PEE:H42	1.90	0.53
41:s:87:VAL:HG23	41:s:88:PRO:CD	2.36	0.53
22:Y:40:ILE:HG23	22:Y:49:GLN:HB2	1.91	0.53
26:c:127:ASN:O	26:c:131:LYS:HG3	2.09	0.53
43:v:78:LEU:HD23	43:v:78:LEU:H	1.74	0.53
12:M:169:VAL:HG21	12:M:222:ILE:HD11	1.90	0.53
12:M:406:ASN:ND2	12:M:688:GLN:O	2.37	0.53
34:k:37:MET:HG3	34:k:67:ALA:CB	2.39	0.53
53:l:701:CDL:H271	47:l:704:PEE:H28	1.90	0.53
1:A:125:CYS:H	1:A:277:ASN:ND2	2.07	0.52
53:N:201:CDL:H711	41:s:43:TYR:HH	1.73	0.52
6:X:85:TYR:OH	23:Z:22:TRP:NE1	2.34	0.52
25:b:32:GLU:HG3	39:p:115:TYR:HA	1.89	0.52
28:e:109:LEU:HD22	40:r:43:ASN:HB2	1.91	0.52
36:m:3:MET:HE2	36:m:3:MET:H	1.74	0.52
43:v:78:LEU:H	43:v:78:LEU:CD2	2.22	0.52
1:A:132:ARG:HB3	1:A:165:GLU:HB3	1.90	0.52
26:c:128:THR:O	26:c:132:HIS:CD2	2.62	0.52
30:g:32:ARG:O	30:g:36:MET:HG2	2.09	0.52
35:l:66:TRP:HB2	47:l:704:PEE:C14	2.39	0.52
39:p:136:GLU:OE1	39:p:167:TRP:NE1	2.42	0.52
1:A:123:GLY:HA2	14:O:180:CYS:CB	2.40	0.52
4:E:68:MET:HA	4:E:68:MET:HE2	1.90	0.52
12:M:408:ARG:HD2	12:M:439:THR:HG23	1.91	0.52
6:X:123:GLU:OE2	39:p:25:ARG:NH2	2.42	0.52
48:a:202:PLX:O1	48:a:202:PLX:H1A2	2.09	0.52
47:i:402:PEE:H27	35:l:563:PRO:HA	1.92	0.52
35:l:66:TRP:CD2	47:l:704:PEE:H19	2.44	0.52
16:Q:450:ILE:O	16:Q:454:GLN:HG3	2.08	0.52
21:W:74:LEU:O	21:W:78:GLU:HG3	2.09	0.52
32:i:268:GLN:HG3	42:u:168:PHE:HZ	1.73	0.52
41:s:51:ASP:HB3	55:s:401:UQ:H8	1.92	0.52
12:M:372:PHE:H	12:M:532:PRO:HB2	1.73	0.52
53:l:701:CDL:H652	48:r:503:PLX:H122	1.90	0.52
43:v:83:GLU:OE1	43:v:83:GLU:N	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:107:GLN:NE2	15:P:136:ARG:HG2	2.24	0.52
16:Q:121:GLU:OE2	16:Q:463:ARG:NH1	2.42	0.52
37:n:56:THR:HG1	37:n:57:TRP:CD1	2.28	0.52
1:A:326:LEU:HD23	1:A:367:ILE:HD11	1.92	0.52
3:C:115:PRO:HG3	15:P:219:VAL:HG21	1.91	0.52
4:E:84:ILE:HG22	4:E:88:MET:HE3	1.92	0.52
9:J:108:TRP:HE3	9:J:116:ILE:HG12	1.75	0.52
16:Q:181:LEU:HD21	16:Q:210:MET:HB2	1.92	0.52
41:s:32:GLN:OE1	41:s:34:ARG:NH2	2.40	0.52
44:w:75:ARG:HB2	44:w:75:ARG:CZ	2.40	0.52
1:A:86:ARG:HD3	1:A:339:PHE:CE2	2.44	0.52
3:C:190:LEU:CD2	47:j:201:PEE:H14	2.40	0.52
31:h:97:HIS:HA	31:h:102:GLU:HB3	1.91	0.52
32:i:88:LYS:HD2	32:i:148:SER:OG	2.09	0.52
44:w:62:VAL:HG12	44:w:70:LYS:HB2	1.92	0.52
12:M:36:VAL:HB	12:M:56:VAL:HG21	1.91	0.52
14:O:156:LEU:HD11	14:O:169:PHE:HD2	1.75	0.52
20:V:53:VAL:HA	20:V:56:THR:HG22	1.92	0.52
20:V:123:ALA:O	20:V:127:MET:HG3	2.09	0.52
32:i:12:THR:HG21	36:m:163:ILE:HG21	1.91	0.52
35:l:37:LYS:HD3	35:l:98:TRP:HE1	1.75	0.52
35:l:66:TRP:HB2	47:l:704:PEE:H20	1.92	0.52
42:u:83:THR:HA	42:u:86:TRP:CD1	2.45	0.52
1:A:392:MET:HE3	1:A:419:ILE:HD12	1.91	0.52
1:A:418:GLN:O	1:A:422:HIS:ND1	2.43	0.52
45:C:301:SF4:S4	16:Q:223:HIS:CD2	3.03	0.52
19:U:26:GLY:HA3	47:U:101:PEE:H37	1.92	0.52
32:i:4:ILE:HD11	44:w:44:VAL:HG13	1.92	0.51
34:k:57:ASN:HB3	36:m:143:ILE:HG13	1.91	0.51
44:w:118:TYR:OH	56:w:401:ADP:O2'	2.28	0.51
9:J:84:TYR:N	9:J:84:TYR:CD1	2.78	0.51
33:j:69:ILE:HD11	41:s:144:VAL:HG13	1.92	0.51
34:k:98:CYS:HB2	35:l:580:GLN:HB2	1.93	0.51
35:l:316:THR:OG1	35:l:395:ILE:HD12	2.10	0.51
40:r:22:MET:HG2	40:r:26:ASN:ND2	2.26	0.51
44:w:169:PHE:HD2	56:w:401:ADP:N1	2.02	0.51
8:I:40:LYS:HB3	21:W:7:LYS:H	1.76	0.51
13:N:127:TYR:OH	18:T:61:GLU:O	2.25	0.51
22:Y:43:ARG:HG3	22:Y:48:PRO:HA	1.92	0.51
35:l:125:LEU:O	35:l:129:MET:HG2	2.10	0.51
14:O:104:ILE:HG22	14:O:105:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:209:GLU:HG2	15:P:224:VAL:HA	1.92	0.51
32:i:20:VAL:HG11	32:i:137:ALA:HB1	1.93	0.51
35:l:15:LEU:HD11	35:l:94:LEU:HD21	1.92	0.51
35:l:86:SER:O	35:l:90:ILE:HG12	2.10	0.51
40:r:115:LEU:HD12	40:r:174:LEU:HD22	1.93	0.51
12:M:591:GLU:HG3	12:M:610:VAL:HG23	1.92	0.51
14:O:146:ASP:OD1	14:O:147:SER:N	2.44	0.51
16:Q:292:MET:HE3	16:Q:454:GLN:HA	1.92	0.51
21:W:30:LEU:HD23	21:W:35:MET:HG2	1.92	0.51
47:i:402:PEE:H28	47:i:402:PEE:H35	1.93	0.51
40:r:357:THR:O	40:r:361:VAL:HG23	2.11	0.51
1:A:62:TRP:CD2	1:A:181:LEU:HD13	2.45	0.51
35:l:250:SER:HB2	35:l:333:ALA:HA	1.91	0.51
40:r:45:LEU:HD22	40:r:50:LEU:CD2	2.40	0.51
40:r:175:ASN:O	40:r:179:ILE:HG12	2.10	0.51
44:w:169:PHE:CG	56:w:401:ADP:C6	2.97	0.51
36:m:55:MET:HA	36:m:55:MET:HE2	1.93	0.51
40:r:57:PHE:CE1	40:r:113:THR:HA	2.46	0.51
44:w:243:LYS:HD3	44:w:243:LYS:N	2.26	0.51
16:Q:176:GLU:OE2	16:Q:311:TYR:OH	2.21	0.51
53:a:201:CDL:C21	53:a:201:CDL:C25	2.86	0.51
44:w:114:LEU:CD2	56:w:401:ADP:H1'	2.40	0.51
1:A:56:ALA:HB1	1:A:61:ASP:HB2	1.93	0.51
6:X:69:SER:OG	6:X:70:ASP:N	2.43	0.51
53:a:201:CDL:OA4	25:b:89:HIS:HE1	1.94	0.51
35:l:86:SER:OG	35:l:262:ARG:NH2	2.44	0.51
35:l:207:GLU:O	35:l:207:GLU:HG2	2.11	0.51
39:p:26:HIS:CD2	39:p:79:PRO:HB3	2.45	0.51
41:s:18:ALA:HB2	55:s:401:UQ:C15	2.41	0.51
7:H:69:GLU:HG3	7:H:77:ILE:HG12	1.92	0.51
19:U:38:TYR:HB2	41:s:310:MET:O	2.11	0.51
53:g:202:CDL:H262	53:g:202:CDL:H332	1.93	0.51
47:i:402:PEE:C25	47:i:402:PEE:C21	2.86	0.51
35:l:309:GLN:O	35:l:313:MET:HG3	2.11	0.51
12:M:379:THR:HG21	12:M:526:LEU:HD22	1.94	0.50
47:m:201:PEE:H2	47:m:201:PEE:H9	1.93	0.50
3:C:191:ARG:HG2	3:C:191:ARG:HH11	1.76	0.50
9:J:129:LEU:HD23	9:J:167:ILE:HG13	1.93	0.50
11:L:111:LEU:HG	11:L:112:MET:HG2	1.94	0.50
16:Q:204:PHE:CD1	16:Q:207:ARG:HD3	2.46	0.50
32:i:130:LEU:HD12	32:i:134:GLN:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:m:35:VAL:O	36:m:39:VAL:HG23	2.11	0.50
9:J:153:ALA:HB2	9:J:191:VAL:HG23	1.92	0.50
12:M:140:GLN:HG2	16:Q:379:ILE:HG12	1.94	0.50
12:M:224:ASP:OD2	12:M:291:ARG:NH2	2.39	0.50
14:O:197:THR:H	14:O:200:ASP:HB3	1.75	0.50
15:P:232:LYS:NZ	15:P:234:ASP:OD1	2.44	0.50
30:g:36:MET:HE1	48:g:201:PLX:H381	1.92	0.50
2:B:63:TRP:HZ2	47:B:303:PEE:H14	1.76	0.50
6:G:83:VAL:O	6:G:87:LEU:HD13	2.12	0.50
12:M:308:ARG:NH2	12:M:578:PRO:O	2.40	0.50
12:M:498:GLN:HB2	12:M:669:ASN:ND2	2.18	0.50
32:i:100:MET:HE1	35:l:595:ILE:HG23	1.94	0.50
40:r:195:MET:HB2	47:r:501:PEE:O4	2.11	0.50
44:w:75:ARG:HH11	44:w:75:ARG:CB	2.24	0.50
6:G:75:THR:C	6:G:77:GLU:H	2.19	0.50
12:M:373:PRO:HG2	12:M:490:LEU:CD2	2.41	0.50
14:O:206:ASP:OD1	14:O:207:GLU:N	2.44	0.50
16:Q:41:VAL:O	16:Q:45:GLU:HG2	2.12	0.50
32:i:54:GLU:HG2	34:k:96:LEU:HD12	1.93	0.50
32:i:153:LEU:O	32:i:157:MET:HG3	2.12	0.50
40:r:369:LEU:HD12	40:r:370:PRO:HD2	1.92	0.50
2:B:63:TRP:HE1	47:B:303:PEE:H1	1.76	0.50
17:S:54:ILE:HD11	31:h:106:PRO:HB3	1.93	0.50
19:U:42:ALA:HB2	41:s:312:ALA:HA	1.94	0.50
22:Y:62:SER:OG	35:l:371:THR:OG1	2.29	0.50
24:a:82:VAL:HG11	28:e:104:THR:HG21	1.93	0.50
35:l:78:LEU:HD11	53:l:701:CDL:H251	1.93	0.50
12:M:488:ALA:HB2	12:M:677:GLN:HB2	1.94	0.50
16:Q:53:TYR:N	16:Q:54:PRO:HD3	2.27	0.50
16:Q:303:ARG:HG3	16:Q:401:GLU:HB3	1.92	0.50
1:A:173:ILE:HG23	1:A:182:ILE:HD11	1.93	0.50
2:B:41:VAL:HA	8:I:113:LEU:HD12	1.93	0.50
6:G:84:LEU:O	6:G:88:LYS:HG2	2.12	0.50
48:a:202:PLX:O4	48:a:202:PLX:O7	2.27	0.50
32:i:95:MET:CE	32:i:149:ILE:CG2	2.89	0.50
34:k:23:ARG:HD3	36:m:23:LYS:HB2	1.93	0.50
53:l:701:CDL:H312	53:l:701:CDL:H761	1.94	0.50
41:s:84:THR:O	41:s:87:VAL:HG22	2.11	0.50
43:v:38:GLU:O	43:v:39:MET:HE2	2.11	0.50
1:A:296:LEU:HG	1:A:337:MET:HE2	1.94	0.50
4:E:40:TYR:HB3	6:G:120:MET:HE1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:105:ARG:NH1	11:L:167:ASN:O	2.40	0.50
12:M:545:LEU:HB3	12:M:566:ILE:HD13	1.93	0.50
31:h:105:ARG:NH2	42:u:17:GLU:OE2	2.30	0.50
47:l:704:PEE:O5	47:l:704:PEE:H1	2.11	0.50
36:m:25:SER:O	36:m:27:ILE:N	2.45	0.50
40:r:418:LYS:HE2	40:r:419:TYR:CE2	2.47	0.50
41:s:96:ILE:HG22	41:s:98:MET:HG3	1.93	0.50
44:w:209:VAL:HG22	44:w:260:ALA:HB2	1.92	0.50
12:M:482:GLN:HA	12:M:482:GLN:OE1	2.12	0.49
13:N:2:GLU:HG3	13:N:4:VAL:HG22	1.94	0.49
49:X:201:8Q1:O3	39:p:13:GLN:NE2	2.45	0.49
48:a:202:PLX:H282	48:a:202:PLX:H321	1.92	0.49
32:i:268:GLN:HG3	42:u:168:PHE:CZ	2.47	0.49
35:l:61:MET:O	35:l:62:ILE:HD13	2.12	0.49
40:r:201:MET:HA	40:r:204:MET:HB2	1.94	0.49
13:N:3:LEU:HD12	53:N:201:CDL:OA7	2.11	0.49
31:h:7:GLN:O	31:h:11:GLY:N	2.45	0.49
40:r:119:TYR:CD1	40:r:119:TYR:C	2.90	0.49
43:v:112:LYS:C	43:v:112:LYS:CD	2.85	0.49
1:A:311:TRP:O	1:A:329:LYS:NZ	2.39	0.49
6:G:126:PHE:CG	6:G:148:ILE:HD11	2.48	0.49
12:M:624:ARG:NH1	12:M:628:GLU:OE2	2.31	0.49
14:O:182:ASN:HD21	14:O:218:PRO:HB3	1.78	0.49
16:Q:136:PHE:HE2	16:Q:409:VAL:HG11	1.77	0.49
22:Y:60:PHE:O	22:Y:64:THR:HG23	2.11	0.49
32:i:7:THR:O	32:i:11:MET:HG2	2.11	0.49
44:w:87:PRO:O	44:w:142:GLN:NE2	2.41	0.49
28:e:77:ASP:OD1	28:e:78:LYS:N	2.46	0.49
35:l:350:LEU:HD23	35:l:350:LEU:O	2.13	0.49
43:v:69:CYS:SG	43:v:70:LYS:N	2.85	0.49
6:G:113:LEU:O	6:G:117:GLU:HG3	2.12	0.49
9:J:204:SER:OG	9:J:238:GLN:O	2.27	0.49
17:S:17:PHE:CE1	41:s:257:ILE:HA	2.47	0.49
18:T:79:VAL:HG21	18:T:84:ILE:HD13	1.94	0.49
48:a:202:PLX:C32	48:a:202:PLX:C28	2.85	0.49
41:s:9:LEU:HD22	41:s:95:LEU:HD12	1.93	0.49
1:A:123:GLY:N	14:O:180:CYS:SG	2.76	0.49
6:G:114:ASP:O	6:G:118:ILE:HG12	2.12	0.49
15:P:130:TYR:HB2	15:P:143:VAL:HB	1.95	0.49
19:U:56:PRO:HG2	42:u:45:LEU:HB2	1.95	0.49
24:a:155:GLU:OE2	24:a:158:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:k:38:LEU:O	34:k:42:ILE:HG12	2.12	0.49
53:n:101:CDL:H261	40:r:6:ILE:CD1	2.42	0.49
44:w:75:ARG:HB2	44:w:75:ARG:HH11	1.75	0.49
1:A:149:MET:HE3	1:A:241:THR:HB	1.95	0.49
12:M:250:SER:OG	12:M:251:ILE:N	2.46	0.49
20:V:102:GLY:HA2	20:V:110:ILE:HG23	1.94	0.49
22:Y:105:ASP:N	22:Y:105:ASP:OD1	2.46	0.49
35:l:292:ALA:HB2	35:l:304:PHE:HB3	1.95	0.49
44:w:39:GLY:HA2	44:w:296:MET:HE1	1.93	0.49
44:w:129:TYR:CD1	44:w:183:CYS:HB3	2.46	0.49
44:w:168:VAL:HG12	44:w:241:TYR:HA	1.94	0.49
1:A:35:LEU:HD23	1:A:40:ARG:HH11	1.77	0.49
10:K:73:TYR:CZ	10:K:75:ASN:HB3	2.47	0.49
16:Q:242:ASP:OD1	21:W:16:TYR:OH	2.26	0.49
24:a:143:GLU:HG3	40:r:175:ASN:ND2	2.18	0.49
41:s:95:LEU:C	41:s:95:LEU:CD2	2.85	0.49
44:w:75:ARG:NH1	44:w:75:ARG:CB	2.73	0.49
44:w:169:PHE:CE2	56:w:401:ADP:N1	2.73	0.49
16:Q:206:GLU:OE2	16:Q:209:LYS:NZ	2.46	0.49
20:V:2:ALA:HA	35:l:601:LEU:HD12	1.95	0.49
53:l:701:CDL:H241	47:l:704:PEE:H33	1.93	0.49
2:B:78:PHE:O	8:I:12:ARG:NH2	2.45	0.49
2:B:89:GLU:HG2	13:N:58:ARG:HA	1.95	0.49
3:C:127:PRO:O	41:s:58:LYS:NZ	2.46	0.49
12:M:381:LEU:HD13	12:M:664:TYR:HB3	1.95	0.49
19:U:14:ALA:O	19:U:15:LYS:HG2	2.13	0.49
19:U:41:TYR:O	19:U:45:ILE:HG13	2.13	0.49
23:Z:32:VAL:HG13	39:p:39:TYR:HB2	1.95	0.49
40:r:44:GLN:HE21	40:r:63:ALA:HB2	1.78	0.49
5:F:68:ARG:NH2	12:M:364:ASP:OD1	2.46	0.48
16:Q:354:GLY:H	21:W:8:GLN:HE22	1.61	0.48
30:g:60:LEU:HD13	44:w:353:TRP:HB2	1.94	0.48
32:i:284:MET:CE	47:i:402:PEE:H46	2.43	0.48
44:w:169:PHE:O	44:w:173:MET:HG3	2.14	0.48
6:G:140:CYS:SG	6:G:143:GLU:HG3	2.53	0.48
9:J:206:ILE:H	50:J:401:NDP:H71N	1.60	0.48
48:g:201:PLX:H1C2	31:h:2:PRO:HD2	1.95	0.48
35:l:327:LEU:O	35:l:331:MET:HG2	2.13	0.48
53:l:701:CDL:H541	53:l:701:CDL:HA61	1.95	0.48
37:n:11:HIS:HA	37:n:14:HIS:HD2	1.78	0.48
12:M:409:PHE:HB2	12:M:688:GLN:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:184:ILE:HD11	16:Q:251:PHE:HZ	1.78	0.48
17:S:17:PHE:HE1	41:s:257:ILE:HA	1.77	0.48
26:c:58:ARG:NH1	38:o:36:ARG:HE	2.11	0.48
48:g:201:PLX:H301	32:i:347:ASN:HB3	1.94	0.48
47:j:201:PEE:H82	55:s:401:UQ:H172	1.95	0.48
48:j:202:PLX:H322	48:j:202:PLX:H381	1.95	0.48
35:l:237:MET:HE3	35:l:303:ALA:HB2	1.96	0.48
40:r:57:PHE:HE1	40:r:113:THR:HA	1.78	0.48
1:A:208:GLU:OE1	1:A:210:THR:OG1	2.27	0.48
2:B:79:ARG:NH1	8:I:25:GLN:OE1	2.45	0.48
12:M:149:ASP:HA	16:Q:380:HIS:CE1	2.48	0.48
24:a:67:PHE:CE2	40:r:434:ASN:HB3	2.48	0.48
37:n:17:VAL:HB	37:n:18:PRO:HD3	1.95	0.48
40:r:158:LEU:HB2	40:r:159:PRO:HD3	1.93	0.48
40:r:436:LEU:O	40:r:440:HIS:ND1	2.39	0.48
13:N:71:ARG:HG3	13:N:73:THR:HG22	1.95	0.48
34:k:6:MET:O	34:k:10:MET:HG3	2.13	0.48
35:l:241:THR:HG21	35:l:344:GLY:HA3	1.96	0.48
35:l:526:LEU:HD12	35:l:530:PRO:HG2	1.94	0.48
1:A:48:ARG:NH1	10:K:70:ASN:O	2.34	0.48
12:M:222:ILE:HA	12:M:225:ILE:HG12	1.96	0.48
26:c:140:MET:HE1	35:l:411:MET:SD	2.54	0.48
35:l:546:GLN:HB2	40:r:278:ARG:HD3	1.96	0.48
1:A:49:HIS:HA	10:K:74:ARG:HD2	1.96	0.48
9:J:109:ASN:CG	9:J:112:ASP:HB2	2.38	0.48
12:M:373:PRO:HG2	12:M:490:LEU:HD22	1.95	0.48
12:M:381:LEU:HD12	12:M:668:ALA:HB2	1.95	0.48
28:e:109:LEU:CD2	40:r:43:ASN:HB2	2.43	0.48
32:i:106:LEU:HG	32:i:138:PRO:HB2	1.94	0.48
35:l:161:ARG:NH1	35:l:238:GLU:OE2	2.47	0.48
35:l:468:ILE:O	35:l:472:ILE:HG12	2.13	0.48
35:l:591:PHE:O	35:l:594:THR:CG2	2.58	0.48
1:A:46:TYR:CD2	14:O:234:LEU:HD12	2.49	0.48
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.54	0.48
21:W:51:MET:HA	41:s:313:SER:HB2	1.95	0.48
6:X:137:LYS:HG3	25:b:4:TYR:HE1	1.77	0.48
34:k:23:ARG:HG2	36:m:23:LYS:HE2	1.95	0.48
35:l:290:LEU:O	35:l:293:ILE:HG22	2.14	0.48
35:l:400:ASN:HD22	35:l:409:LEU:HD11	1.78	0.48
35:l:559:GLU:O	35:l:563:PRO:HD2	2.12	0.48
35:l:591:PHE:CA	35:l:594:THR:HG22	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:l:704:PEE:H8	47:l:704:PEE:P	2.54	0.48
37:n:19:VAL:O	37:n:22:VAL:HG22	2.14	0.48
39:p:13:GLN:HE22	39:p:17:LEU:HD11	1.78	0.48
40:r:12:LEU:HB2	40:r:13:PRO:HD3	1.96	0.48
40:r:300:ALA:O	40:r:308:SER:HB3	2.14	0.48
41:s:102:VAL:HG13	41:s:150:LEU:HD21	1.95	0.48
44:w:96:SER:HA	44:w:101:GLY:HA2	1.95	0.48
4:E:16:SER:HB3	11:L:52:LEU:HB3	1.95	0.48
11:L:89:SER:O	12:M:59:GLN:NE2	2.47	0.48
47:U:101:PEE:C21	41:s:302:MET:HE1	2.43	0.48
21:W:125:TYR:HB3	21:W:133:ILE:HG12	1.96	0.48
36:m:124:ASP:OD1	36:m:124:ASP:N	2.45	0.48
44:w:170:LEU:HD12	44:w:179:ILE:CD1	2.44	0.48
12:M:29:SER:OG	12:M:30:ASN:N	2.46	0.48
16:Q:387:GLU:OE2	16:Q:390:GLN:NE2	2.45	0.48
32:i:153:LEU:HD13	35:l:602:PHE:CE2	2.48	0.48
32:i:211:MET:HG2	32:i:333:SER:HB2	1.95	0.48
40:r:188:ASN:OD1	40:r:256:TYR:OH	2.20	0.48
1:A:177:TYR:HB3	10:K:96:PHE:HD2	1.79	0.47
4:E:28:ALA:O	4:E:32:VAL:HG23	2.13	0.47
32:i:288:LEU:HD23	47:i:402:PEE:H55	1.96	0.47
33:j:6:THR:HG21	41:s:87:VAL:HG11	1.94	0.47
35:l:1:MET:SD	35:l:1:MET:C	2.97	0.47
35:l:174:TYR:CD2	35:l:232:TRP:HB3	2.49	0.47
53:l:702:CDL:H541	53:l:702:CDL:H572	1.61	0.47
42:u:106:LYS:O	42:u:109:GLU:HG3	2.14	0.47
1:A:210:THR:HB	1:A:224:ARG:HG2	1.95	0.47
5:F:24:CYS:O	5:F:34:ARG:NH1	2.47	0.47
12:M:275:PRO:HB3	12:M:286:ILE:HG23	1.96	0.47
15:P:119:VAL:HG12	15:P:121:THR:HG22	1.96	0.47
21:W:93:GLU:HG3	31:h:98:HIS:NE2	2.29	0.47
6:X:120:MET:HE1	39:p:24:LEU:HB2	1.96	0.47
35:l:592:LEU:O	35:l:596:MET:HG3	2.14	0.47
7:H:81:ILE:HG22	7:H:85:GLU:OE2	2.14	0.47
9:J:170:LEU:HA	9:J:202:LYS:HB3	1.95	0.47
47:m:201:PEE:C30	41:s:98:MET:HE3	2.44	0.47
43:v:22:MET:HE1	43:v:102:PHE:CE1	2.50	0.47
1:A:129:GLU:OE1	1:A:287:THR:OG1	2.22	0.47
6:G:75:THR:O	6:G:78:ALA:N	2.47	0.47
9:J:37:HIS:CE1	18:T:49:ASP:HA	2.49	0.47
12:M:370:GLU:HG2	12:M:482:GLN:HE22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:156:LEU:HD12	14:O:164:THR:HG21	1.96	0.47
15:P:213:ASP:HB3	15:P:216:VAL:HG22	1.96	0.47
26:c:125:SER:O	26:c:129:MET:HG3	2.15	0.47
27:d:89:GLU:O	27:d:93:ARG:HG2	2.15	0.47
32:i:95:MET:HE3	32:i:149:ILE:CG2	2.43	0.47
39:p:44:MET:O	39:p:48:PHE:HB2	2.13	0.47
40:r:45:LEU:HD23	40:r:45:LEU:N	2.30	0.47
44:w:116:LYS:NZ	44:w:123:SER:OG	2.47	0.47
44:w:123:SER:OG	44:w:125:ASP:OD1	2.28	0.47
3:C:126:GLU:O	3:C:128:ARG:N	2.48	0.47
20:V:102:GLY:O	20:V:106:ARG:N	2.47	0.47
26:c:155:PRO:HG3	43:v:4:HIS:CE1	2.49	0.47
7:H:64:ASP:OD1	7:H:65:VAL:N	2.46	0.47
16:Q:107:ARG:HA	16:Q:107:ARG:HD3	1.71	0.47
25:b:9:LYS:O	25:b:13:GLN:HG2	2.14	0.47
32:i:95:MET:CE	32:i:149:ILE:HA	2.45	0.47
35:l:307:SER:HA	35:l:310:LEU:HD12	1.97	0.47
40:r:158:LEU:N	40:r:159:PRO:HD2	2.30	0.47
11:L:174:THR:HG21	14:O:114:GLU:OE1	2.15	0.47
12:M:301:ARG:HD2	12:M:301:ARG:HA	1.71	0.47
6:X:81:ASP:HB3	23:Z:16:LEU:HD22	1.97	0.47
24:a:127:ASP:OD1	48:a:202:PLX:C1	2.63	0.47
26:c:139:PHE:CD2	53:l:702:CDL:H861	2.50	0.47
33:j:49:LEU:N	33:j:50:PRO:HD2	2.30	0.47
35:l:4:PHE:CD1	35:l:4:PHE:C	2.92	0.47
36:m:163:ILE:O	36:m:167:VAL:HG23	2.15	0.47
37:n:7:ILE:O	37:n:11:HIS:N	2.47	0.47
42:u:83:THR:HA	42:u:86:TRP:NE1	2.28	0.47
1:A:129:GLU:CD	1:A:287:THR:CG2	2.80	0.47
1:A:211:ALA:HB2	1:A:223:PRO:HG3	1.97	0.47
4:E:127:ASP:OD1	11:L:104:ARG:NH1	2.48	0.47
9:J:163:LYS:HG2	9:J:259:LYS:HZ3	1.80	0.47
9:J:203:PRO:O	50:J:401:NDP:H5N	2.15	0.47
16:Q:293:LEU:HD22	16:Q:298:ILE:HD12	1.97	0.47
30:g:48:ASN:HB3	30:g:55:VAL:HA	1.96	0.47
35:l:97:THR:HG21	35:l:125:LEU:HD22	1.97	0.47
47:r:501:PEE:H21	47:r:501:PEE:H28	1.59	0.47
12:M:318:THR:HG23	12:M:321:ASP:H	1.79	0.47
12:M:394:VAL:HG11	12:M:418:ILE:HG12	1.97	0.47
20:V:42:ALA:HB2	35:l:593:ILE:CD1	2.43	0.47
28:e:90:VAL:HG22	40:r:28:THR:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ASN:HA	1:A:359:ARG:NH2	2.30	0.47
2:B:98:ARG:CZ	16:Q:220:ALA:HB2	2.45	0.47
2:B:205:ILE:O	2:B:209:TYR:HB3	2.14	0.47
6:X:111:ASP:OD1	6:X:112:SER:N	2.48	0.47
32:i:11:MET:CE	32:i:11:MET:CA	2.87	0.47
40:r:116:ILE:HG13	42:u:168:PHE:CD1	2.50	0.47
41:s:21:THR:HB	55:s:401:UQ:HM23	1.96	0.47
9:J:127:ILE:HD11	9:J:253:ILE:HD11	1.97	0.46
12:M:64:CYS:O	12:M:184:ARG:NH2	2.38	0.46
12:M:306:MET:HE1	13:N:139:PRO:HG3	1.96	0.46
6:X:75:THR:OG1	6:X:156:GLU:O	2.28	0.46
35:l:557:TRP:O	35:l:561:ILE:HG12	2.15	0.46
53:l:702:CDL:H622	53:l:702:CDL:H591	1.58	0.46
48:r:502:PLX:H92	48:r:502:PLX:H121	1.70	0.46
44:w:175:ARG:HG2	44:w:175:ARG:HH11	1.80	0.46
1:A:244:ASN:ND2	46:A:502:FMN:O2	2.29	0.46
3:C:50:LEU:CD1	47:j:201:PEE:C17	2.76	0.46
4:E:23:ARG:HH11	4:E:23:ARG:HG2	1.80	0.46
4:E:96:VAL:HG12	4:E:96:VAL:O	2.15	0.46
7:H:35:LEU:HD11	7:H:48:THR:HG22	1.97	0.46
9:J:65:LEU:HD23	9:J:129:LEU:HD22	1.96	0.46
9:J:251:ASN:O	9:J:255:ASP:N	2.44	0.46
12:M:48:THR:HA	12:M:95:PRO:HA	1.96	0.46
31:h:29:ILE:HD11	36:m:136:PHE:HE1	1.81	0.46
32:i:17:THR:O	32:i:21:MET:HG3	2.15	0.46
20:V:140:LYS:NZ	24:a:158:ARG:HG3	2.30	0.46
24:a:87:THR:HG23	53:a:201:CDL:OA7	2.15	0.46
53:a:201:CDL:H191	53:a:201:CDL:H732	1.98	0.46
25:b:86:LEU:HD11	35:l:9:LEU:HD12	1.97	0.46
33:j:3:ILE:HG22	47:m:201:PEE:H13	1.96	0.46
33:j:4:MET:HE3	47:m:201:PEE:C15	2.46	0.46
33:j:103:ALA:O	33:j:107:THR:HG23	2.15	0.46
35:l:102:GLU:OE2	35:l:456:ARG:NH2	2.47	0.46
35:l:384:PRO:HD3	35:l:491:LEU:HD11	1.96	0.46
40:r:14:MET:HE2	40:r:30:HIS:ND1	2.29	0.46
44:w:290:THR:HG22	44:w:293:ARG:HH21	1.80	0.46
1:A:41:ILE:HG21	1:A:250:VAL:HG12	1.96	0.46
12:M:198:THR:HG21	12:M:209:TYR:HB2	1.96	0.46
14:O:200:ASP:CG	14:O:219:ARG:HG3	2.38	0.46
16:Q:80:LEU:HD23	16:Q:80:LEU:H	1.81	0.46
35:l:267:MET:O	35:l:274:GLN:NE2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:457:PRO:HG2	40:r:458:LEU:HD12	1.96	0.46
14:O:159:LYS:HB2	14:O:162:GLU:HG3	1.98	0.46
16:Q:226:TYR:OH	16:Q:234:GLN:O	2.23	0.46
1:A:121:GLU:HG3	1:A:122:PRO:HD2	1.98	0.46
9:J:168:SER:OG	9:J:188:GLU:OE1	2.27	0.46
12:M:382:ARG:NH1	12:M:527:ASP:OD2	2.49	0.46
12:M:402:LEU:HD23	12:M:475:VAL:HB	1.97	0.46
32:i:111:PHE:HA	35:l:591:PHE:CE1	2.50	0.46
32:i:283:ALA:HB1	40:r:158:LEU:HD13	1.96	0.46
53:n:101:CDL:H121	53:n:101:CDL:C27	2.45	0.46
42:u:103:GLN:N	42:u:103:GLN:OE1	2.46	0.46
3:C:188:LYS:HD3	3:C:191:ARG:NE	2.31	0.46
4:E:119:LEU:HD11	12:M:628:GLU:HG2	1.98	0.46
10:K:79:HIS:CD2	14:O:215:LYS:HB2	2.51	0.46
16:Q:102:SER:O	16:Q:102:SER:OG	2.31	0.46
26:c:139:PHE:CE2	53:l:702:CDL:H841	2.51	0.46
34:k:45:THR:HG23	36:m:52:LEU:HD13	1.96	0.46
40:r:216:LEU:HD23	40:r:287:ALA:HB1	1.97	0.46
1:A:125:CYS:HB2	1:A:277:ASN:HD21	1.79	0.46
3:C:133:MET:HG2	3:C:168:PRO:HG2	1.97	0.46
5:F:46:LYS:HE3	12:M:674:LEU:HD11	1.97	0.46
9:J:271:TYR:OH	9:J:346:GLU:OE1	2.20	0.46
12:M:370:GLU:HG2	12:M:482:GLN:NE2	2.30	0.46
16:Q:198:THR:HB	16:Q:199:PRO:HD3	1.98	0.46
24:a:115:HIS:NE2	53:a:201:CDL:OB4	2.49	0.46
28:e:76:TYR:HB2	28:e:83:ASP:OD1	2.16	0.46
32:i:284:MET:HE2	47:i:402:PEE:H46	1.98	0.46
33:j:3:ILE:HG21	47:m:201:PEE:H13	1.97	0.46
35:l:3:PRO:HG2	35:l:53:MET:CE	2.46	0.46
3:C:103:MET:HE3	3:C:124:MET:HE3	1.97	0.46
12:M:33:GLU:HB3	12:M:98:LYS:HE2	1.98	0.46
14:O:59:ASN:ND2	14:O:89:GLN:OE1	2.49	0.46
16:Q:148:GLU:HB3	16:Q:227:ILE:HB	1.98	0.46
53:a:201:CDL:H521	47:l:704:PEE:C11	2.46	0.46
35:l:33:PRO:HB3	35:l:118:PHE:CZ	2.51	0.46
53:n:101:CDL:H252	53:n:101:CDL:H221	1.71	0.46
40:r:74:PRO:O	40:r:78:MET:HG3	2.16	0.46
44:w:258:TYR:CE2	44:w:269:VAL:HG22	2.51	0.46
9:J:243:VAL:O	9:J:247:LYS:HG3	2.16	0.46
10:K:107:SER:OG	10:K:110:HIS:ND1	2.37	0.46
12:M:698:ASP:OD1	12:M:698:ASP:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:137:THR:HG22	14:O:138:THR:H	1.80	0.46
32:i:38:LEU:HD12	34:k:73:LEU:HD22	1.98	0.46
35:l:536:LEU:HB3	35:l:537:PRO:HD3	1.98	0.46
40:r:22:MET:O	40:r:26:ASN:ND2	2.49	0.46
41:s:2:PHE:CE1	41:s:95:LEU:HD21	2.51	0.46
41:s:9:LEU:O	41:s:13:ILE:HG12	2.15	0.46
44:w:295:ARG:HA	44:w:298:VAL:HG22	1.97	0.46
1:A:317:VAL:HG23	1:A:356:VAL:HG12	1.98	0.45
1:A:332:CYS:HA	1:A:335:VAL:HG12	1.97	0.45
8:I:96:THR:HB	8:I:97:PRO:HD2	1.97	0.45
21:W:85:GLN:OE1	31:h:105:ARG:HD2	2.16	0.45
24:a:119:ARG:O	24:a:123:ARG:HG2	2.16	0.45
35:l:66:TRP:CD1	47:l:704:PEE:H18	2.51	0.45
35:l:338:MET:HE2	35:l:338:MET:HB3	1.83	0.45
36:m:23:LYS:N	36:m:24:PRO:HD3	2.31	0.45
43:v:22:MET:HE1	43:v:102:PHE:CD1	2.51	0.45
44:w:40:PRO:O	44:w:44:VAL:HG23	2.16	0.45
1:A:185:ASN:C	1:A:187:CYS:H	2.24	0.45
1:A:199:ARG:NH1	14:O:84:ASP:OD2	2.40	0.45
12:M:638:THR:O	12:M:642:VAL:HG23	2.16	0.45
39:p:28:GLU:HB3	39:p:37:TYR:CE1	2.51	0.45
4:E:121:LYS:HA	4:E:124:VAL:HG22	1.99	0.45
15:P:211:ARG:HH12	15:P:213:ASP:HB2	1.81	0.45
16:Q:315:GLU:O	16:Q:346:GLN:NE2	2.34	0.45
32:i:43:VAL:HG11	32:i:129:LEU:HD23	1.98	0.45
33:j:95:LEU:HD13	41:s:302:MET:HG3	1.98	0.45
34:k:2:PRO:HD2	34:k:5:TYR:CD2	2.51	0.45
34:k:43:MET:HE3	34:k:47:ILE:HD11	1.97	0.45
47:m:201:PEE:H9	47:m:201:PEE:C1	2.46	0.45
40:r:33:LEU:O	40:r:37:ILE:HG12	2.17	0.45
41:s:140:ILE:O	41:s:143:GLU:HG2	2.16	0.45
43:v:93:LEU:O	43:v:97:LYS:HG3	2.16	0.45
44:w:330:LYS:HA	44:w:330:LYS:HD2	1.79	0.45
12:M:680:LEU:CD1	12:M:680:LEU:N	2.80	0.45
25:b:4:TYR:HB3	25:b:9:LYS:HG2	1.98	0.45
26:c:83:GLN:HA	26:c:86:ARG:HG3	1.98	0.45
28:e:102:GLY:CA	40:r:39:LEU:HD23	2.46	0.45
32:i:62:THR:HG21	32:i:114:TRP:CD1	2.50	0.45
38:o:17:THR:O	38:o:23:TYR:OH	2.26	0.45
40:r:166:TYR:O	40:r:170:THR:HG23	2.16	0.45
40:r:231:LEU:HA	40:r:235:LEU:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:GLU:O	1:A:451:GLN:HG3	2.16	0.45
9:J:131:GLY:HA3	50:J:401:NDP:O3D	2.17	0.45
12:M:385:TYR:OH	12:M:527:ASP:OD1	2.24	0.45
13:N:122:GLN:HA	18:T:59:GLN:HG2	1.99	0.45
16:Q:187:VAL:HG11	16:Q:258:LEU:HD21	1.99	0.45
30:g:2:THR:HG22	30:g:4:MET:HG3	1.99	0.45
53:l:701:CDL:H241	47:l:704:PEE:C21	2.46	0.45
40:r:373:ILE:HA	40:r:376:ILE:HD12	1.98	0.45
5:F:30:SER:HB2	5:F:34:ARG:HH12	1.81	0.45
11:L:92:ASN:HB3	15:P:238:PRO:HA	1.99	0.45
12:M:354:LEU:HD22	12:M:548:LEU:HD22	1.99	0.45
12:M:422:TRP:HA	12:M:427:LEU:HB3	1.99	0.45
15:P:147:THR:HB	15:P:153:ILE:HD11	1.97	0.45
16:Q:188:THR:HG21	16:Q:203:MET:HB2	1.99	0.45
16:Q:251:PHE:HB3	16:Q:341:LEU:HD11	1.99	0.45
16:Q:295:GLY:HA2	16:Q:321:GLY:HA3	1.98	0.45
53:a:201:CDL:H531	47:l:704:PEE:H56	1.96	0.45
32:i:326:LEU:HB3	32:i:327:PRO:HD3	1.99	0.45
39:p:138:LYS:O	39:p:142:GLU:HG2	2.16	0.45
43:v:63:LEU:CD1	43:v:67:LEU:HD11	2.47	0.45
1:A:146:GLY:HA3	1:A:193:PHE:CE1	2.52	0.45
3:C:126:GLU:N	41:s:59:GLU:OE2	2.47	0.45
12:M:278:HIS:CE1	12:M:280:ASP:HB2	2.52	0.45
36:m:7:PHE:O	36:m:11:THR:HG23	2.17	0.45
37:n:27:LEU:HD21	53:n:101:CDL:C12	2.47	0.45
43:v:76:ASN:OD1	43:v:78:LEU:HD23	2.16	0.45
44:w:146:ALA:HB1	44:w:157:VAL:HG21	1.99	0.45
1:A:269:ARG:HB2	1:A:269:ARG:HH11	1.81	0.45
2:B:180:HIS:CE1	9:J:100:LEU:HD11	2.52	0.45
3:C:84:TYR:CE1	3:C:171:GLU:HG2	2.52	0.45
12:M:261:ILE:HG22	12:M:286:ILE:HG21	1.99	0.45
12:M:266:ARG:HB3	12:M:271:MET:HE3	1.98	0.45
12:M:640:ASP:OD1	12:M:641:GLN:N	2.50	0.45
13:N:21:ARG:HB3	13:N:21:ARG:NH1	2.31	0.45
16:Q:371:MET:HE3	16:Q:371:MET:HB3	1.91	0.45
16:Q:431:HIS:O	16:Q:454:GLN:NE2	2.46	0.45
53:a:201:CDL:OA4	25:b:89:HIS:CE1	2.70	0.45
25:b:12:LEU:HD23	25:b:16:ARG:NH2	2.32	0.45
26:c:96:ASP:OD1	26:c:96:ASP:N	2.47	0.45
32:i:175:LEU:O	32:i:179:MET:HG2	2.17	0.45
33:j:33:LYS:HD2	33:j:33:LYS:C	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:136:ASN:HD21	47:l:704:PEE:H45	1.81	0.45
35:l:331:MET:HB3	35:l:387:THR:HG22	1.99	0.45
21:W:36:PHE:O	21:W:40:ILE:HG12	2.17	0.45
24:a:106:VAL:HG11	37:n:47:ARG:HD2	1.98	0.45
28:e:152:ASP:OD1	28:e:153:GLU:N	2.48	0.45
53:n:101:CDL:H812	53:n:101:CDL:H781	1.84	0.45
1:A:392:MET:O	1:A:396:MET:HG2	2.17	0.45
14:O:191:ASN:C	14:O:191:ASN:ND2	2.70	0.45
22:Y:50:LEU:HB3	22:Y:55:LEU:HD11	1.97	0.45
24:a:131:LYS:NZ	37:n:32:ASP:OD2	2.27	0.45
53:n:101:CDL:H781	53:n:101:CDL:H752	1.68	0.45
5:F:41:TYR:CZ	5:F:55:ILE:HD11	2.52	0.44
11:L:163:ASN:O	11:L:171:ARG:HA	2.17	0.44
12:M:124:HIS:HD2	16:Q:375:MET:HE2	1.82	0.44
12:M:387:LEU:C	12:M:514:ASN:OD1	2.60	0.44
14:O:208:LEU:HD23	14:O:208:LEU:HA	1.89	0.44
6:X:119:ILE:HG21	6:X:135:ALA:HB1	1.99	0.44
25:b:5:THR:OG1	25:b:8:GLU:HG3	2.16	0.44
32:i:26:TRP:HB3	32:i:74:ILE:HD13	1.98	0.44
35:l:313:MET:HG2	35:l:328:HIS:HD2	1.81	0.44
47:l:704:PEE:H31	40:r:449:LEU:HD23	1.99	0.44
53:n:101:CDL:H712	53:n:101:CDL:H741	1.66	0.44
38:o:65:LEU:HD11	40:r:343:ILE:HD11	1.99	0.44
40:r:346:ARG:O	40:r:419:TYR:HA	2.18	0.44
9:J:80:VAL:C	9:J:81:ILE:HD12	2.42	0.44
17:S:45:TRP:CD1	21:W:140:PHE:HB2	2.52	0.44
53:a:201:CDL:H512	47:l:704:PEE:C33	2.47	0.44
32:i:200:MET:SD	32:i:265:MET:HB3	2.57	0.44
34:k:26:LEU:HD12	34:k:29:SER:HB2	1.97	0.44
2:B:179:THR:OG1	2:B:182:GLU:OE2	2.36	0.44
8:I:18:ARG:HH12	16:Q:256:ASP:HB3	1.82	0.44
9:J:88:PRO:O	9:J:89:TYR:C	2.61	0.44
15:P:52:ASP:O	15:P:56:LYS:HG3	2.17	0.44
28:e:102:GLY:CA	40:r:39:LEU:CD2	2.95	0.44
33:j:24:LEU:CD2	47:j:201:PEE:H67	2.48	0.44
35:l:66:TRP:CB	47:l:704:PEE:C14	2.96	0.44
12:M:389:THR:O	12:M:390:THR:OG1	2.29	0.44
15:P:140:ARG:NH2	16:Q:406:GLU:OE2	2.49	0.44
39:p:63:LEU:O	39:p:64:LEU:HB3	2.16	0.44
40:r:306:PRO:HA	40:r:458:LEU:HD22	1.98	0.44
41:s:24:GLU:HA	41:s:271:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:371:VAL:HG22	12:M:533:GLY:HA2	1.99	0.44
14:O:130:TYR:HA	14:O:189:ASN:ND2	2.31	0.44
6:X:106:LYS:HE2	6:X:106:LYS:HB3	1.86	0.44
6:X:113:LEU:O	6:X:117:GLU:HG3	2.18	0.44
23:Z:25:GLU:HA	23:Z:30:GLU:OE2	2.18	0.44
25:b:109:THR:O	27:d:19:ALA:N	2.51	0.44
35:l:384:PRO:HA	35:l:389:PHE:CG	2.51	0.44
44:w:175:ARG:HG2	44:w:175:ARG:NH1	2.33	0.44
1:A:174:ARG:HG3	10:K:93:LEU:HG	1.99	0.44
9:J:106:MET:HE1	18:T:53:VAL:CG2	2.43	0.44
12:M:217:GLU:HG3	12:M:412:PRO:HB3	2.00	0.44
14:O:130:TYR:CE2	14:O:208:LEU:HD22	2.52	0.44
16:Q:236:LEU:HD22	16:Q:240:LEU:HD23	2.00	0.44
27:d:109:ARG:NH2	27:d:131:GLN:OE1	2.51	0.44
30:g:110:THR:O	30:g:114:ILE:HG13	2.17	0.44
36:m:170:GLU:OE2	36:m:173:ARG:NH1	2.51	0.44
40:r:39:LEU:HD12	40:r:39:LEU:HA	1.77	0.44
42:u:38:LYS:HB3	42:u:39:PRO:HD3	1.98	0.44
1:A:244:ASN:N	46:A:502:FMN:O1P	2.39	0.44
48:C:302:PLX:H281	48:C:302:PLX:H311	1.63	0.44
10:K:106:GLN:H	10:K:106:GLN:CD	2.26	0.44
11:L:62:THR:HG23	11:L:72:ILE:HD13	1.99	0.44
26:c:58:ARG:HH12	38:o:36:ARG:HE	1.66	0.44
53:i:401:CDL:H132	53:i:401:CDL:C17	2.45	0.44
35:l:33:PRO:HB3	35:l:118:PHE:CE1	2.53	0.44
39:p:108:HIS:CD2	39:p:109:PRO:HD2	2.53	0.44
41:s:14:LEU:HA	41:s:17:VAL:HG22	2.00	0.44
1:A:278:ILE:HD11	1:A:299:LEU:HD21	1.99	0.44
3:C:55:ASN:ND2	3:C:187:GLU:O	2.50	0.44
47:U:101:PEE:H59	47:U:101:PEE:H64	1.77	0.44
23:Z:49:GLU:OE2	39:p:38:ARG:NH1	2.43	0.44
26:c:38:PRO:HB2	38:o:75:ASN:ND2	2.31	0.44
31:h:21:GLN:HA	34:k:53:PHE:CE1	2.53	0.44
32:i:237:MET:HE3	32:i:237:MET:HB2	1.93	0.44
35:l:66:TRP:CG	47:l:704:PEE:C14	3.00	0.44
35:l:172:ILE:HG21	40:r:408:LEU:HD12	2.00	0.44
44:w:258:TYR:HE2	44:w:269:VAL:HG22	1.83	0.44
9:J:116:ILE:HG22	9:J:155:VAL:HG21	1.99	0.44
10:K:109:ARG:HG2	10:K:109:ARG:HH11	1.83	0.44
24:a:60:SER:HB3	39:p:107:TRP:HA	1.99	0.44
36:m:10:SER:O	36:m:14:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:22:MET:HG2	40:r:26:ASN:HD21	1.83	0.44
21:W:93:GLU:O	21:W:97:ILE:HG13	2.17	0.43
21:W:128:ARG:HB3	21:W:132:GLU:OE2	2.18	0.43
25:b:12:LEU:HD23	25:b:16:ARG:HH22	1.83	0.43
47:l:704:PEE:C4	47:l:704:PEE:H2	2.48	0.43
38:o:102:TYR:HB2	40:r:263:MET:HG3	1.99	0.43
39:p:76:HIS:O	39:p:78:GLN:N	2.51	0.43
43:v:68:LYS:HE3	43:v:68:LYS:HB3	1.89	0.43
1:A:133:HIS:CD2	10:K:75:ASN:ND2	2.86	0.43
1:A:235:VAL:HG12	1:A:240:THR:OG1	2.17	0.43
3:C:191:ARG:HG2	3:C:191:ARG:NH1	2.33	0.43
13:N:10:GLY:O	13:N:14:VAL:HG23	2.18	0.43
6:X:122:MET:HE1	6:X:144:ILE:HG21	2.00	0.43
35:l:368:PHE:HB3	35:l:445:GLU:OE2	2.18	0.43
42:u:49:GLU:OE1	42:u:135:ARG:NH2	2.51	0.43
44:w:132:GLN:NE2	44:w:166:ASP:OD1	2.51	0.43
2:B:74:LEU:HB2	41:s:272:TRP:CZ2	2.53	0.43
12:M:266:ARG:HD2	12:M:267:THR:HG23	2.00	0.43
12:M:351:LEU:O	12:M:530:TYR:OH	2.29	0.43
14:O:44:THR:HG22	14:O:46:GLU:H	1.84	0.43
24:a:110:TRP:CG	24:a:123:ARG:HB3	2.53	0.43
53:a:201:CDL:H512	47:l:704:PEE:H53	2.01	0.43
25:b:10:LEU:HG	25:b:14:GLN:HE21	1.84	0.43
32:i:177:LYS:NZ	34:k:97:GLN:O	2.45	0.43
32:i:278:MET:HB3	32:i:279:PRO:HD3	1.99	0.43
47:l:703:PEE:H64	47:l:703:PEE:H22	2.00	0.43
40:r:123:GLU:OE2	40:r:157:SER:OG	2.26	0.43
40:r:253:LEU:HD12	40:r:256:TYR:CE1	2.53	0.43
40:r:371:PRO:O	40:r:448:THR:OG1	2.32	0.43
44:w:169:PHE:CE2	56:w:401:ADP:C5	3.05	0.43
44:w:279:ASP:OD1	44:w:279:ASP:N	2.50	0.43
9:J:64:PHE:CE2	9:J:242:ILE:HD13	2.54	0.43
12:M:43:VAL:HG12	12:M:55:LYS:HD2	2.01	0.43
22:Y:76:ASP:O	35:l:385:TYR:OH	2.21	0.43
26:c:133:LEU:HD22	26:c:133:LEU:C	2.43	0.43
29:f:59:ILE:O	29:f:63:LYS:HG2	2.18	0.43
32:i:230:LEU:HD11	32:i:244:MET:HE1	2.01	0.43
53:l:701:CDL:H311	53:l:701:CDL:H561	2.00	0.43
53:l:701:CDL:H651	53:l:701:CDL:H841	2.00	0.43
38:o:14:LEU:HD12	38:o:15:PRO:HD2	2.01	0.43
40:r:196:TRP:CE3	40:r:257:MET:HE3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:LEU:HD23	1:A:40:ARG:NH1	2.33	0.43
1:A:372:GLU:HG2	1:A:376:HIS:CE1	2.54	0.43
2:B:191:LEU:HB3	18:T:63:ASN:ND2	2.34	0.43
32:i:217:MET:HB3	32:i:326:LEU:HD13	1.98	0.43
35:l:166:THR:HG22	47:l:703:PEE:H2	1.96	0.43
39:p:100:PRO:HG3	40:r:419:TYR:CE1	2.52	0.43
1:A:99:TRP:N	1:A:99:TRP:CD1	2.86	0.43
2:B:99:GLY:HA3	2:B:170:GLY:O	2.19	0.43
5:F:83:SER:OG	5:F:86:GLN:HG3	2.19	0.43
26:c:183:HIS:ND1	43:v:58:TYR:OH	2.51	0.43
53:g:202:CDL:H862	53:g:202:CDL:H832	1.84	0.43
32:i:31:ILE:HD11	34:k:62:ILE:HG21	1.99	0.43
32:i:71:MET:O	32:i:75:ILE:HG12	2.19	0.43
47:i:402:PEE:C22	47:i:402:PEE:C18	2.86	0.43
35:l:66:TRP:CB	47:l:704:PEE:H19	2.49	0.43
35:l:213:LEU:HB3	35:l:273:VAL:HG11	2.01	0.43
40:r:190:TRP:CZ2	48:r:502:PLX:H11	2.54	0.43
41:s:14:LEU:HA	41:s:17:VAL:CG2	2.49	0.43
1:A:133:HIS:NE2	10:K:75:ASN:ND2	2.65	0.43
1:A:201:ALA:HB1	14:O:121:MET:HB2	1.99	0.43
21:W:85:GLN:O	21:W:89:GLU:HG3	2.19	0.43
33:j:70:ALA:HB2	36:m:59:ILE:HG13	2.00	0.43
35:l:338:MET:HB2	35:l:457:LEU:HB3	2.00	0.43
38:o:48:LEU:HB3	39:p:166:LEU:HD13	1.99	0.43
1:A:162:PHE:HZ	14:O:178:GLY:HA3	1.84	0.43
3:C:146:SER:OG	16:Q:118:2MR:O	2.21	0.43
4:E:23:ARG:HG2	4:E:23:ARG:NH1	2.33	0.43
12:M:544:VAL:HG23	12:M:565:PHE:HD2	1.83	0.43
21:W:63:GLU:OE1	42:u:119:ARG:NH2	2.52	0.43
27:d:105:ILE:O	27:d:109:ARG:HG3	2.18	0.43
35:l:304:PHE:CZ	35:l:526:LEU:HD22	2.54	0.43
47:l:704:PEE:H16	47:l:704:PEE:H22	1.77	0.43
43:v:78:LEU:HD23	43:v:78:LEU:N	2.34	0.43
44:w:169:PHE:CD2	56:w:401:ADP:C2	3.01	0.43
8:I:46:SER:HB2	16:Q:359:ASP:OD2	2.19	0.43
12:M:403:VAL:HG12	12:M:432:ILE:HD12	2.00	0.43
16:Q:39:PRO:HB3	16:Q:43:TRP:CD1	2.53	0.43
16:Q:82:LEU:HD12	16:Q:101:LEU:HD12	2.01	0.43
20:V:91:PHE:HE1	20:V:120:LEU:HD22	1.84	0.43
53:a:201:CDL:H422	53:a:201:CDL:H381	2.01	0.43
30:g:122:ARG:CZ	38:o:116:ILE:HG21	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:288:LEU:HD21	35:l:570:GLN:HG3	1.99	0.43
48:j:202:PLX:H131	48:j:202:PLX:H182	2.01	0.43
47:l:704:PEE:O5	47:l:704:PEE:H53	2.19	0.43
15:P:183:ASP:OD1	15:P:183:ASP:N	2.52	0.43
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.54	0.43
23:Z:57:PHE:CD1	35:l:435:PRO:HG3	2.53	0.43
25:b:28:LEU:HG	25:b:32:GLU:HG2	1.99	0.43
26:c:176:LYS:HD2	26:c:176:LYS:HA	1.76	0.43
31:h:2:PRO:HB2	31:h:3:PHE:H	1.70	0.43
36:m:45:LEU:HD23	36:m:50:SER:HA	2.00	0.43
1:A:141:GLY:HA3	1:A:248:VAL:O	2.19	0.42
12:M:204:MET:HE3	12:M:204:MET:HB2	1.88	0.42
12:M:467:LYS:HE3	12:M:503:SER:HB2	2.01	0.42
12:M:696:MET:SD	12:M:702:ARG:HA	2.59	0.42
16:Q:198:THR:HG22	16:Q:202:TRP:CE2	2.54	0.42
17:S:43:TYR:CZ	21:W:68:ARG:HG3	2.54	0.42
17:S:57:VAL:HG23	17:S:59:ARG:HB2	2.00	0.42
21:W:121:MET:HE2	36:m:129:ASP:O	2.19	0.42
23:Z:24:ILE:O	23:Z:27:THR:OG1	2.22	0.42
25:b:81:ILE:CG2	47:l:704:PEE:H58	2.46	0.42
26:c:160:GLN:HG2	26:c:183:HIS:CD2	2.54	0.42
33:j:3:ILE:HD13	47:m:201:PEE:H51	2.00	0.42
33:j:90:MET:SD	36:m:151:THR:HG23	2.59	0.42
35:l:417:SER:HB2	35:l:493:VAL:HG22	2.00	0.42
53:l:701:CDL:H392	53:l:701:CDL:H341	2.00	0.42
40:r:44:GLN:HG3	40:r:60:SER:HA	2.01	0.42
40:r:48:ASN:OD1	40:r:48:ASN:N	2.52	0.42
16:Q:53:TYR:HE2	47:i:402:PEE:O2P	2.02	0.42
19:U:81:LEU:O	21:W:59:ARG:NH1	2.53	0.42
47:U:101:PEE:H35	47:U:101:PEE:H30	1.47	0.42
28:e:116:GLU:O	28:e:120:ARG:HG3	2.19	0.42
31:h:68:LEU:HD23	31:h:68:LEU:HA	1.90	0.42
32:i:247:THR:O	32:i:251:MET:HG3	2.18	0.42
33:j:3:ILE:CD1	47:m:201:PEE:C32	2.92	0.42
35:l:100:ILE:HG21	35:l:246:LEU:HB2	2.01	0.42
35:l:362:LEU:HB3	35:l:366:MET:HG2	2.01	0.42
53:l:701:CDL:H801	48:r:503:PLX:H212	2.00	0.42
40:r:18:SER:HB2	40:r:23:ILE:HG22	2.00	0.42
48:r:502:PLX:H51	48:r:502:PLX:H6	1.31	0.42
2:B:85:ASN:HB3	2:B:89:GLU:OE1	2.19	0.42
9:J:113:LYS:HE2	9:J:113:LYS:HB3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:186:ARG:NH1	15:P:189:THR:OG1	2.52	0.42
6:X:82:ARG:HD2	22:Y:44:TYR:CE1	2.54	0.42
32:i:72:MET:HE3	34:k:12:PHE:CG	2.53	0.42
32:i:112:HIS:HB2	32:i:184:ILE:HD13	2.01	0.42
32:i:245:MET:HE3	32:i:245:MET:HB3	1.89	0.42
32:i:265:MET:HE3	32:i:265:MET:HA	2.01	0.42
43:v:92:HIS:O	43:v:96:VAL:HG23	2.19	0.42
48:C:302:PLX:H212	48:C:302:PLX:H181	1.70	0.42
9:J:82:VAL:HA	9:J:83:PRO:HD3	1.83	0.42
12:M:712:LYS:HD3	12:M:712:LYS:N	2.34	0.42
13:N:59:HIS:CD2	13:N:60:ARG:HG3	2.54	0.42
13:N:65:THR:O	13:N:73:THR:OG1	2.35	0.42
14:O:129:LYS:HG3	14:O:130:TYR:CD1	2.55	0.42
18:T:38:VAL:HG22	18:T:44:ALA:HB2	2.01	0.42
31:h:84:ASP:HA	31:h:87:ILE:HG22	2.00	0.42
35:l:49:VAL:HB	35:l:50:PRO:HD3	2.01	0.42
35:l:562:LEU:HB2	35:l:563:PRO:HD3	2.01	0.42
53:n:101:CDL:C12	53:n:101:CDL:C27	2.98	0.42
41:s:14:LEU:O	41:s:17:VAL:HG23	2.18	0.42
41:s:85:MET:SD	41:s:233:MET:HE2	2.60	0.42
1:A:129:GLU:OE1	1:A:287:THR:HG21	2.19	0.42
1:A:325:PRO:HG3	1:A:433:TRP:HB3	2.02	0.42
13:N:3:LEU:O	13:N:6:VAL:HG22	2.19	0.42
27:d:80:LYS:HA	27:d:80:LYS:HD3	1.69	0.42
35:l:103:PHE:HB2	35:l:341:MET:HE3	2.01	0.42
47:l:703:PEE:O5	47:l:703:PEE:H1	2.18	0.42
44:w:170:LEU:HD22	44:w:187:TYR:CG	2.55	0.42
1:A:372:GLU:CG	1:A:376:HIS:HE1	2.32	0.42
13:N:106:ARG:HB2	13:N:109:ILE:HG13	2.01	0.42
16:Q:63:PRO:HA	16:Q:64:PRO:HD3	1.81	0.42
16:Q:196:ALA:O	16:Q:197:MET:HG2	2.20	0.42
6:X:113:LEU:HA	6:X:116:VAL:HG12	2.01	0.42
24:a:141:GLN:O	24:a:145:GLU:HG3	2.19	0.42
40:r:4:ILE:CD1	40:r:41:LEU:HD11	2.50	0.42
40:r:127:VAL:HB	40:r:128:PRO:HD3	2.00	0.42
40:r:337:VAL:HG12	40:r:339:SER:HB3	2.01	0.42
41:s:179:TRP:CG	41:s:180:PRO:HD3	2.54	0.42
1:A:41:ILE:HG22	1:A:137:LYS:NZ	2.35	0.42
1:A:385:CYS:O	1:A:389:VAL:HB	2.20	0.42
2:B:118:LEU:HD11	16:Q:382:PHE:CE2	2.55	0.42
13:N:8:ARG:HA	13:N:8:ARG:HD3	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:199:PRO:HA	16:Q:202:TRP:HB2	2.00	0.42
48:a:202:PLX:H22	48:a:202:PLX:H1C3	1.82	0.42
27:d:33:LEU:HD13	35:l:49:VAL:HG13	2.02	0.42
27:d:90:MET:HE3	27:d:90:MET:HB3	1.88	0.42
32:i:44:LEU:HD22	32:i:122:ILE:HG21	2.02	0.42
34:k:82:SER:O	34:k:86:GLY:N	2.47	0.42
47:m:201:PEE:C1	47:m:201:PEE:C4	2.98	0.42
53:n:101:CDL:H521	53:n:101:CDL:H551	1.89	0.42
38:o:57:LEU:O	38:o:57:LEU:HG	2.20	0.42
44:w:295:ARG:O	44:w:299:GLN:HG2	2.19	0.42
2:B:88:PHE:CZ	13:N:30:ALA:HA	2.54	0.42
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.53	0.42
3:C:188:LYS:HD2	3:C:191:ARG:HH21	1.84	0.42
9:J:167:ILE:HD13	9:J:201:ILE:HB	2.01	0.42
12:M:133:GLN:O	12:M:137:CYS:HB2	2.20	0.42
16:Q:372:LYS:NZ	18:T:94:GLY:O	2.46	0.42
18:T:69:ASP:O	18:T:73:GLU:HG3	2.18	0.42
27:d:65:HIS:ND1	28:e:120:ARG:HD2	2.34	0.42
48:g:201:PLX:H1C3	48:g:201:PLX:H22	1.73	0.42
35:l:2:ASN:N	35:l:3:PRO:CD	2.83	0.42
1:A:43:THR:HG21	14:O:238:PRO:HB3	2.02	0.42
3:C:188:LYS:HG3	3:C:188:LYS:O	2.19	0.42
48:C:302:PLX:H252	48:C:302:PLX:H52	1.76	0.42
4:E:101:THR:O	4:E:105:ARG:HG3	2.20	0.42
5:F:53:ILE:N	12:M:380:ASP:OD1	2.52	0.42
15:P:44:ARG:NE	15:P:45:PRO:HD3	2.33	0.42
34:k:1:MET:HE3	34:k:5:TYR:HB2	2.01	0.42
35:l:268:GLU:HA	35:l:274:GLN:HE22	1.85	0.42
35:l:345:SER:HB2	35:l:450:LEU:HD11	2.02	0.42
35:l:505:ASN:O	35:l:508:THR:HG22	2.20	0.42
53:l:702:CDL:H661	53:l:702:CDL:H452	2.02	0.42
39:p:19:LEU:HD22	39:p:64:LEU:HD12	2.02	0.42
1:A:102:MET:HE2	1:A:111:LYS:HE3	2.02	0.42
8:I:8:ILE:HD11	53:N:201:CDL:H142	2.02	0.42
11:L:156:LYS:HE2	12:M:68:ARG:HD2	2.02	0.42
12:M:144:MET:HG3	16:Q:383:LYS:HG3	2.00	0.42
12:M:690:THR:HG22	12:M:691:ILE:N	2.35	0.42
14:O:141:MET:HE2	14:O:141:MET:HB3	1.94	0.42
16:Q:440:LYS:HD3	16:Q:440:LYS:HA	1.88	0.42
21:W:88:ARG:O	21:W:92:GLU:HG2	2.19	0.42
22:Y:84:PHE:HB3	43:v:92:HIS:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:62:TYR:OH	26:c:74:ASP:OD1	2.36	0.42
26:c:164:ASN:HA	26:c:181:VAL:HG12	2.02	0.42
32:i:10:ILE:O	32:i:14:MET:HG3	2.20	0.42
32:i:310:ASN:HB2	44:w:309:THR:HG22	2.02	0.42
40:r:318:ALA:HB1	40:r:374:ASN:OD1	2.20	0.42
41:s:152:SER:HA	41:s:155:LEU:HD12	2.01	0.42
55:s:401:UQ:H152	55:s:401:UQ:H121	1.90	0.42
1:A:372:GLU:CG	1:A:376:HIS:CE1	3.03	0.41
6:G:104:PHE:HB3	6:G:110:LEU:HB2	2.02	0.41
12:M:541:PRO:HA	12:M:542:PRO:HD3	1.86	0.41
14:O:225:CYS:SG	14:O:225:CYS:O	2.78	0.41
21:W:43:LEU:HG	41:s:179:TRP:HE1	1.84	0.41
22:Y:93:THR:O	22:Y:97:LEU:HD23	2.20	0.41
23:Z:13:LYS:HD2	23:Z:13:LYS:HA	1.79	0.41
47:l:704:PEE:H60	47:l:704:PEE:H55	1.88	0.41
40:r:4:ILE:HD12	40:r:41:LEU:HD11	2.02	0.41
42:u:134:ASP:OD1	42:u:134:ASP:C	2.63	0.41
4:E:94:ILE:HD13	4:E:94:ILE:HA	1.87	0.41
5:F:40:ARG:NH2	5:F:84:ALA:HB1	2.28	0.41
6:G:69:SER:N	16:Q:60:HIS:ND1	2.67	0.41
11:L:158:LYS:NZ	12:M:69:LEU:O	2.40	0.41
31:h:94:PRO:HA	31:h:95:PRO:HD3	1.90	0.41
32:i:95:MET:HE2	32:i:149:ILE:HA	2.00	0.41
35:l:1:MET:SD	35:l:1:MET:O	2.78	0.41
35:l:233:LEU:HB3	35:l:234:PRO:HD3	2.01	0.41
40:r:106:LEU:HD13	40:r:234:VAL:HG11	2.02	0.41
40:r:129:THR:HG21	40:r:231:LEU:HD21	2.02	0.41
40:r:436:LEU:HG	40:r:440:HIS:HE1	1.85	0.41
41:s:293:PHE:O	41:s:297:THR:OG1	2.24	0.41
2:B:144:ARG:HB2	13:N:130:THR:HG23	2.02	0.41
3:C:196:ARG:CB	9:J:85:ARG:HH11	2.28	0.41
9:J:71:ASN:HB2	9:J:97:MET:SD	2.60	0.41
12:M:398:ASP:OD1	12:M:398:ASP:N	2.53	0.41
14:O:196:LEU:HD23	14:O:201:ILE:HB	2.02	0.41
26:c:55:TYR:OH	26:c:74:ASP:O	2.25	0.41
32:i:314:LYS:HE3	44:w:305:LEU:O	2.20	0.41
35:l:428:PHE:HA	35:l:432:LEU:HD12	2.03	0.41
39:p:100:PRO:HG3	40:r:419:TYR:CZ	2.56	0.41
40:r:303:ILE:HG22	40:r:305:THR:HG23	2.02	0.41
1:A:395:VAL:HG11	1:A:412:LEU:HD13	2.01	0.41
2:B:141:ARG:HD3	2:B:141:ARG:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:83:PRO:HB2	9:J:108:TRP:CG	2.55	0.41
9:J:182:ARG:O	9:J:186:VAL:HG23	2.21	0.41
9:J:279:TYR:CD2	9:J:371:PRO:HA	2.55	0.41
16:Q:361:ALA:HA	16:Q:364:SER:O	2.20	0.41
19:U:33:PRO:HG3	41:s:306:SER:OG	2.20	0.41
49:X:201:8Q1:O33	39:p:13:GLN:HG2	2.20	0.41
27:d:43:ARG:HB3	27:d:44:PRO:HD3	2.02	0.41
31:h:38:LYS:NZ	31:h:39:GLU:OE1	2.54	0.41
41:s:87:VAL:CG2	41:s:88:PRO:CD	2.97	0.41
6:G:103:HIS:H	6:G:107:ASP:HB2	1.86	0.41
12:M:355:LYS:HG3	12:M:366:LEU:HD13	2.00	0.41
24:a:168:TRP:HB3	30:g:2:THR:O	2.20	0.41
53:a:201:CDL:H761	53:a:201:CDL:H191	2.02	0.41
35:l:221:ALA:HA	35:l:226:GLN:HG2	2.03	0.41
41:s:62:ARG:NH1	41:s:64:ALA:HA	2.35	0.41
14:O:196:LEU:HA	14:O:200:ASP:OD2	2.21	0.41
6:X:120:MET:SD	39:p:21:LYS:HG3	2.59	0.41
32:i:226:THR:HG23	32:i:229:SER:H	1.86	0.41
35:l:124:PHE:CE1	35:l:252:MET:HB2	2.54	0.41
35:l:188:TRP:CZ2	35:l:209:PRO:HG2	2.56	0.41
35:l:241:THR:HG21	35:l:344:GLY:CA	2.51	0.41
35:l:264:TYR:HA	35:l:267:MET:HB2	2.03	0.41
44:w:350:LYS:HD3	44:w:350:LYS:HA	1.85	0.41
1:A:134:ASP:N	1:A:135:PRO:HD3	2.36	0.41
1:A:135:PRO:HB2	1:A:172:ALA:CB	2.51	0.41
12:M:296:GLY:O	12:M:572:HIS:NE2	2.33	0.41
12:M:369:GLU:OE1	12:M:369:GLU:N	2.51	0.41
14:O:42:ARG:HH21	18:T:104:LYS:HG3	1.86	0.41
18:T:46:ASP:OD1	18:T:46:ASP:N	2.48	0.41
21:W:144:THR:HB	41:s:96:ILE:HG23	2.02	0.41
24:a:155:GLU:HA	24:a:155:GLU:OE1	2.21	0.41
30:g:45:LEU:HD22	30:g:55:VAL:HG12	2.02	0.41
30:g:110:THR:HG22	30:g:112:GLY:H	1.85	0.41
53:g:202:CDL:H792	53:g:202:CDL:H761	1.87	0.41
35:l:14:ILE:HD11	35:l:43:ALA:HA	2.03	0.41
35:l:96:VAL:O	35:l:100:ILE:HG12	2.21	0.41
35:l:317:ILE:HD13	35:l:317:ILE:HA	1.97	0.41
35:l:396:ILE:HA	35:l:399:VAL:HG12	2.03	0.41
40:r:133:ILE:HD11	40:r:231:LEU:HD11	2.03	0.41
40:r:370:PRO:HD3	40:r:375:LEU:HD22	2.02	0.41
41:s:106:LEU:HD23	41:s:106:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:62:VAL:CG1	44:w:70:LYS:HB2	2.51	0.41
44:w:199:LEU:HD21	44:w:286:GLN:NE2	2.36	0.41
1:A:278:ILE:O	14:O:181:VAL:HG23	2.21	0.41
53:N:201:CDL:H742	53:N:201:CDL:H531	2.01	0.41
14:O:137:THR:HG22	14:O:138:THR:N	2.36	0.41
17:S:12:MET:HE2	41:s:23:VAL:CG2	2.46	0.41
21:W:137:THR:HG23	21:W:138:TYR:CD1	2.56	0.41
23:Z:53:TYR:CE2	35:l:434:LYS:HG3	2.55	0.41
25:b:110:ILE:HG12	27:d:16:ARG:HB2	2.03	0.41
48:j:202:PLX:H312	48:j:202:PLX:H282	1.84	0.41
53:l:702:CDL:H312	53:l:702:CDL:H522	2.03	0.41
40:r:222:GLU:OE2	40:r:222:GLU:HA	2.21	0.41
43:v:83:GLU:H	43:v:83:GLU:CD	2.15	0.41
1:A:177:TYR:HB3	10:K:96:PHE:CD2	2.56	0.41
5:F:82:PHE:HB3	5:F:87:VAL:HG13	2.03	0.41
7:H:59:VAL:HG23	7:H:68:LEU:HD21	2.03	0.41
7:H:77:ILE:HG22	7:H:81:ILE:HD11	2.02	0.41
9:J:57:THR:OG1	9:J:123:SER:OG	2.30	0.41
12:M:496:ILE:O	12:M:500:ILE:HG12	2.21	0.41
13:N:9:ARG:CD	53:N:201:CDL:OB4	2.61	0.41
16:Q:191:ALA:HB1	16:Q:196:ALA:HB3	2.03	0.41
21:W:28:ARG:HA	21:W:28:ARG:HD2	1.85	0.41
6:X:117:GLU:OE2	39:p:45:ARG:NH1	2.54	0.41
24:a:145:GLU:HA	24:a:148:GLU:HG2	2.02	0.41
48:a:202:PLX:H91	48:a:202:PLX:H122	1.86	0.41
26:c:143:MET:HE2	35:l:407:TRP:CZ3	2.56	0.41
48:g:201:PLX:H131	48:g:201:PLX:H102	1.87	0.41
32:i:89:MET:HE3	32:i:95:MET:SD	2.60	0.41
47:j:201:PEE:H72	41:s:56:PHE:CD2	2.55	0.41
35:l:20:MET:HA	48:r:503:PLX:H211	2.03	0.41
35:l:60:GLU:OE1	35:l:83:ASP:HA	2.21	0.41
35:l:108:MET:HE3	35:l:108:MET:HB3	1.92	0.41
53:n:101:CDL:H742	53:n:101:CDL:H162	2.02	0.41
38:o:54:PRO:HG3	39:p:129:ARG:NE	2.36	0.41
40:r:1:MET:HB2	40:r:52:PHE:CD2	2.56	0.41
40:r:44:GLN:NE2	40:r:63:ALA:HB2	2.36	0.41
40:r:45:LEU:CD1	40:r:47:GLU:HB2	2.44	0.41
40:r:173:SER:O	40:r:179:ILE:HD11	2.19	0.41
40:r:185:PRO:HB3	40:r:252:PRO:HD3	2.03	0.41
40:r:337:VAL:HG21	40:r:345:ALA:HB2	2.03	0.41
40:r:365:THR:HG21	40:r:444:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:s:401:UQ:H202	55:s:401:UQ:H171	1.84	0.41
44:w:58:LYS:NZ	44:w:278:CYS:HB2	2.36	0.41
44:w:61:THR:HG23	44:w:201:PRO:CB	2.51	0.41
44:w:192:LYS:HG3	44:w:193:VAL:N	2.35	0.41
1:A:394:LYS:HB3	12:M:155:GLU:HG2	2.02	0.41
46:A:502:FMN:N1	46:A:502:FMN:O3'	2.38	0.41
15:P:103:HIS:CD2	15:P:105:ASN:HB2	2.55	0.41
16:Q:52:MET:HE3	16:Q:52:MET:HB3	1.85	0.41
19:U:14:ALA:C	19:U:16:GLU:H	2.29	0.41
6:X:87:LEU:HD23	6:X:87:LEU:HA	1.89	0.41
6:X:138:LEU:HB3	6:X:144:ILE:HG12	2.02	0.41
25:b:19:ARG:HE	39:p:173:ARG:NH2	2.19	0.41
25:b:75:VAL:O	25:b:79:VAL:HG23	2.21	0.41
32:i:287:LEU:HD23	32:i:287:LEU:HA	1.89	0.41
33:j:3:ILE:HD11	47:m:201:PEE:H50	2.01	0.41
33:j:55:PHE:HB3	36:m:70:TYR:HE2	1.85	0.41
43:v:16:GLU:HB2	43:v:17:PRO:HD2	2.03	0.41
44:w:314:LEU:O	44:w:318:THR:HG22	2.21	0.41
46:A:502:FMN:HM81	46:A:502:FMN:HM73	1.85	0.40
2:B:77:LEU:HD12	41:s:31:MET:HG3	2.03	0.40
3:C:62:LEU:O	3:C:91:VAL:HA	2.20	0.40
7:H:83:GLN:NE2	15:P:107:GLN:OE1	2.54	0.40
9:J:195:PHE:HB3	9:J:198:ALA:HB2	2.03	0.40
12:M:372:PHE:CZ	12:M:385:TYR:HB3	2.56	0.40
14:O:203:GLU:O	14:O:207:GLU:HG2	2.21	0.40
16:Q:51:VAL:O	16:Q:54:PRO:HG3	2.21	0.40
17:S:16:LEU:O	17:S:19:PRO:HD2	2.20	0.40
23:Z:20:LYS:O	23:Z:23:LYS:NZ	2.52	0.40
26:c:143:MET:HB3	35:l:407:TRP:CE2	2.56	0.40
32:i:186:HIS:O	32:i:190:MET:HG3	2.21	0.40
44:w:47:GLU:C	44:w:48:ARG:HD3	2.46	0.40
1:A:165:GLU:HA	1:A:168:ASN:HB2	2.03	0.40
6:G:90:TYR:OH	6:G:114:ASP:OD1	2.35	0.40
9:J:350:ILE:HD11	9:J:357:ARG:HH22	1.86	0.40
16:Q:179:ARG:HG3	16:Q:403:PRO:HB3	2.03	0.40
25:b:10:LEU:HG	25:b:14:GLN:NE2	2.35	0.40
27:d:35:LYS:O	27:d:39:LEU:HD13	2.22	0.40
32:i:261:MET:HB3	32:i:262:PRO:HD3	2.03	0.40
35:l:319:ILE:HG22	35:l:404:THR:HG21	2.04	0.40
36:m:3:MET:HE2	36:m:3:MET:N	2.35	0.40
36:m:25:SER:HB3	36:m:28:TYR:HD2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:203:PHE:HB2	40:r:243:MET:HG3	2.03	0.40
42:u:100:CYS:HB2	42:u:103:GLN:OE1	2.22	0.40
1:A:357:MET:HB3	1:A:361:THR:HG21	2.03	0.40
46:A:502:FMN:H1'1	46:A:502:FMN:H9	1.78	0.40
5:F:41:TYR:OH	5:F:53:ILE:HB	2.20	0.40
9:J:116:ILE:O	9:J:120:VAL:HG22	2.21	0.40
9:J:272:LEU:H	9:J:272:LEU:HD12	1.86	0.40
11:L:80:PHE:HE1	11:L:100:GLU:HG2	1.86	0.40
12:M:370:GLU:CG	12:M:482:GLN:NE2	2.85	0.40
53:N:201:CDL:H312	53:N:201:CDL:C54	2.42	0.40
16:Q:48:GLY:HA2	32:i:228:LEU:HD11	2.02	0.40
21:W:120:MET:H	21:W:123:GLU:HG3	1.85	0.40
22:Y:65:MET:SD	35:l:375:ILE:HG12	2.60	0.40
24:a:156:VAL:CG1	24:a:160:MET:HE3	2.51	0.40
26:c:156:VAL:HG11	43:v:95:TYR:CZ	2.56	0.40
27:d:159:GLN:NE2	28:e:142:PHE:O	2.48	0.40
28:e:84:LEU:HD21	28:e:88:ARG:HH21	1.87	0.40
32:i:10:ILE:HD13	32:i:10:ILE:HA	1.94	0.40
32:i:95:MET:CE	32:i:149:ILE:CA	2.99	0.40
35:l:9:LEU:HD23	35:l:9:LEU:HA	1.80	0.40
41:s:89:LEU:HA	41:s:90:PRO:HD3	1.90	0.40
44:w:270:VAL:O	44:w:273:ILE:HB	2.21	0.40
1:A:132:ARG:CB	1:A:165:GLU:HB2	2.51	0.40
3:C:113:MET:HE3	3:C:116:ALA:HB3	2.04	0.40
4:E:91:GLU:O	4:E:95:ASN:ND2	2.34	0.40
17:S:41:PHE:HB3	36:m:135:PHE:C	2.46	0.40
18:T:78:GLU:OE2	18:T:119:ARG:NH2	2.48	0.40
6:X:85:TYR:O	6:X:89:LEU:HD23	2.21	0.40
26:c:108:ASP:HB3	26:c:111:MET:HE3	2.03	0.40
27:d:43:ARG:O	27:d:47:LEU:HG	2.20	0.40
32:i:190:MET:CE	32:i:205:LEU:HA	2.52	0.40
48:j:202:PLX:H342	48:j:202:PLX:H372	1.85	0.40
36:m:74:MET:HE2	36:m:74:MET:HB3	1.99	0.40
41:s:236:ALA:HB1	41:s:259:PHE:HZ	1.86	0.40
43:v:80:CYS:O	43:v:80:CYS:SG	2.79	0.40
44:w:59:VAL:HG13	44:w:201:PRO:HA	2.04	0.40
1:A:41:ILE:H	1:A:289:GLU:CD	2.30	0.40
1:A:384:PRO:HB2	1:A:423:THR:HG22	2.03	0.40
1:A:392:MET:HE1	1:A:432:ALA:HA	2.03	0.40
2:B:63:TRP:CZ2	47:B:303:PEE:H14	2.57	0.40
2:B:131:GLU:HB2	2:B:144:ARG:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:THR:HG21	2:B:180:HIS:CD2	2.57	0.40
9:J:135:GLU:HG3	9:J:141:PHE:HE1	1.87	0.40
9:J:320:GLU:O	9:J:324:MET:HG3	2.21	0.40
20:V:116:ALA:O	20:V:120:LEU:HD23	2.22	0.40
24:a:50:HIS:HB3	24:a:52:LYS:HE2	2.02	0.40
24:a:140:LEU:HD21	40:r:177:LEU:HB3	2.03	0.40
27:d:126:ALA:O	27:d:130:GLU:HG2	2.22	0.40
30:g:28:LEU:HD23	30:g:28:LEU:HA	1.90	0.40
35:l:173:LEU:HD12	40:r:405:LEU:HD21	2.04	0.40
35:l:332:HIS:HA	35:l:335:PHE:CE2	2.57	0.40
40:r:436:LEU:HG	40:r:440:HIS:CE1	2.56	0.40
41:s:294:LEU:HD12	41:s:294:LEU:HA	1.87	0.40
42:u:61:LYS:O	42:u:65:GLN:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	413 (96%)	16 (4%)	0	100	100
2	B	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
3	C	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
4	E	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
5	F	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
6	G	86/88 (98%)	85 (99%)	0	1 (1%)	10	42
6	X	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
7	H	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
8	I	93/112 (83%)	81 (87%)	12 (13%)	0	100	100
9	J	289/341 (85%)	278 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	K	40/42 (95%)	40 (100%)	0	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	666 (97%)	22 (3%)	0	100	100
13	N	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
14	O	215/217 (99%)	209 (97%)	6 (3%)	0	100	100
15	P	206/208 (99%)	194 (94%)	12 (6%)	0	100	100
16	Q	412/430 (96%)	400 (97%)	11 (3%)	1 (0%)	43	73
17	S	68/70 (97%)	68 (100%)	0	0	100	100
18	T	94/96 (98%)	93 (99%)	1 (1%)	0	100	100
19	U	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
20	V	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	18	52
21	W	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
22	Y	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
23	Z	82/84 (98%)	79 (96%)	3 (4%)	0	100	100
24	a	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
25	b	99/126 (79%)	96 (97%)	3 (3%)	0	100	100
26	c	154/156 (99%)	147 (96%)	7 (4%)	0	100	100
27	d	173/175 (99%)	169 (98%)	4 (2%)	0	100	100
28	e	105/107 (98%)	97 (92%)	8 (8%)	0	100	100
29	f	40/42 (95%)	40 (100%)	0	0	100	100
30	g	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
31	h	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
32	i	345/347 (99%)	334 (97%)	11 (3%)	0	100	100
33	j	95/113 (84%)	88 (93%)	7 (7%)	0	100	100
34	k	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
35	l	601/603 (100%)	575 (96%)	26 (4%)	0	100	100
36	m	125/175 (71%)	113 (90%)	12 (10%)	0	100	100
37	n	54/56 (96%)	54 (100%)	0	0	100	100
38	o	126/128 (98%)	120 (95%)	6 (5%)	0	100	100
39	p	176/178 (99%)	168 (96%)	8 (4%)	0	100	100
40	r	457/459 (100%)	446 (98%)	10 (2%)	1 (0%)	43	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	s	299/318 (94%)	290 (97%)	8 (3%)	1 (0%)	36	68
42	u	169/171 (99%)	162 (96%)	7 (4%)	0	100	100
43	v	122/131 (93%)	117 (96%)	5 (4%)	0	100	100
44	w	318/320 (99%)	303 (95%)	15 (5%)	0	100	100
All	All	8029/8315 (97%)	7732 (96%)	292 (4%)	5 (0%)	49	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	G	76	LEU
40	r	48	ASN
16	Q	229	PRO
20	V	46	PRO
41	s	90	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	345/345 (100%)	343 (99%)	2 (1%)	78	84
2	B	151/151 (100%)	151 (100%)	0	100	100
3	C	132/132 (100%)	132 (100%)	0	100	100
4	E	107/107 (100%)	107 (100%)	0	100	100
5	F	76/76 (100%)	76 (100%)	0	100	100
6	G	66/81 (82%)	66 (100%)	0	100	100
6	X	76/81 (94%)	76 (100%)	0	100	100
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	87 (100%)	0	100	100
9	J	253/295 (86%)	252 (100%)	1 (0%)	84	86
10	K	41/41 (100%)	41 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	L	113/113 (100%)	112 (99%)	1 (1%)	70	81
12	M	579/580 (100%)	576 (100%)	3 (0%)	81	85
13	N	130/130 (100%)	130 (100%)	0	100	100
14	O	180/183 (98%)	179 (99%)	1 (1%)	78	84
15	P	190/190 (100%)	190 (100%)	0	100	100
16	Q	361/370 (98%)	360 (100%)	1 (0%)	86	88
17	S	58/58 (100%)	58 (100%)	0	100	100
18	T	79/79 (100%)	79 (100%)	0	100	100
19	U	69/69 (100%)	69 (100%)	0	100	100
20	V	101/101 (100%)	101 (100%)	0	100	100
21	W	122/123 (99%)	122 (100%)	0	100	100
22	Y	63/63 (100%)	62 (98%)	1 (2%)	55	75
23	Z	65/65 (100%)	65 (100%)	0	100	100
24	a	121/122 (99%)	121 (100%)	0	100	100
25	b	98/119 (82%)	98 (100%)	0	100	100
26	c	141/141 (100%)	140 (99%)	1 (1%)	76	83
27	d	155/155 (100%)	155 (100%)	0	100	100
28	e	99/99 (100%)	99 (100%)	0	100	100
29	f	35/38 (92%)	35 (100%)	0	100	100
30	g	108/108 (100%)	108 (100%)	0	100	100
31	h	93/93 (100%)	93 (100%)	0	100	100
32	i	311/311 (100%)	309 (99%)	2 (1%)	78	84
33	j	88/99 (89%)	88 (100%)	0	100	100
34	k	85/85 (100%)	85 (100%)	0	100	100
35	l	537/537 (100%)	535 (100%)	2 (0%)	84	86
36	m	99/141 (70%)	99 (100%)	0	100	100
37	n	46/53 (87%)	46 (100%)	0	100	100
38	o	113/113 (100%)	113 (100%)	0	100	100
39	p	159/159 (100%)	159 (100%)	0	100	100
40	r	410/410 (100%)	410 (100%)	0	100	100
41	s	263/275 (96%)	263 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	u	153/153 (100%)	153 (100%)	0	100	100
43	v	97/115 (84%)	96 (99%)	1 (1%)	68	80
44	w	282/283 (100%)	282 (100%)	0	100	100
All	All	7036/7238 (97%)	7020 (100%)	16 (0%)	85	89

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	GLU
1	A	131	ILE
9	J	85	ARG
11	L	86	ASN
12	M	471	LYS
12	M	513	MET
12	M	515	ILE
14	O	191	ASN
16	Q	217	VAL
22	Y	46	GLN
26	c	133	LEU
32	i	11	MET
32	i	91	ASN
35	l	11	THR
35	l	594	THR
43	v	69	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	HIS
1	A	277	ASN
1	A	284	HIS
1	A	346	GLN
1	A	418	GLN
1	A	457	HIS
4	E	108	HIS
7	H	21	HIS
7	H	83	GLN
9	J	166	HIS
10	K	100	GLN
12	M	260	ASN

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Mol	Chain	Res	Type
12	M	300	GLN
12	M	460	HIS
12	M	604	GLN
12	M	669	ASN
13	N	116	ASN
14	O	187	GLN
15	P	55	HIS
15	P	77	GLN
15	P	196	HIS
16	Q	60	HIS
16	Q	160	ASN
16	Q	234	GLN
17	S	61	HIS
18	T	123	HIS
20	V	134	GLN
21	W	8	GLN
23	Z	21	GLN
24	a	50	HIS
25	b	89	HIS
25	b	126	GLN
26	c	100	ASN
26	c	132	HIS
26	c	164	ASN
27	d	107	GLN
27	d	149	HIS
31	h	34	HIS
32	i	36	ASN
32	i	91	ASN
32	i	134	GLN
32	i	268	GLN
32	i	310	ASN
32	i	322	GLN
34	k	97	GLN
35	l	72	GLN
35	l	135	ASN
35	l	194	ASN
35	l	199	GLN
35	l	274	GLN
35	l	447	ASN
37	n	14	HIS
38	o	79	ASN
39	p	13	GLN

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Mol	Chain	Res	Type
40	r	26	ASN
40	r	83	HIS
40	r	180	HIS
40	r	251	ASN
40	r	304	GLN
40	r	338	HIS
41	s	247	HIS
41	s	317	GLN
42	u	30	HIS
42	u	35	GLN
43	v	47	ASN
44	w	107	GLN
44	w	344	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	2MR	Q	118	16	10,12,13	1.98	1 (10%)	5,13,15	5.90	3 (60%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	2MR	Q	118	16	-	2/10/13/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.73	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	118	2MR	NE-CZ-NH2	12.04	130.52	119.48
16	Q	118	2MR	CD-NE-CZ	4.31	131.49	123.41
16	Q	118	2MR	CQ2-NH2-CZ	3.11	130.74	123.86

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	Q	118	2MR	NE-CD-CG-CB
16	Q	118	2MR	CA-CB-CG-CD

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	Q	118	2MR	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 37 ligands modelled in this entry, 2 are monoatomic - leaving 35 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	PEE	i	402	-	46,46,50	1.20	6 (13%)	49,51,55	1.01	2 (4%)
45	SF4	C	301	3	0,12,12	-	-	-		
45	SF4	B	302	2	0,12,12	-	-	-		
48	PLX	g	201	-	51,51,51	1.15	4 (7%)	55,59,59	0.59	1 (1%)
49	8Q1	X	201	6	31,34,34	2.16	6 (19%)	40,43,43	1.68	9 (22%)
56	ADP	w	401	-	27,29,29	2.98	8 (29%)	42,45,45	1.96	9 (21%)
49	8Q1	G	201	6	31,34,34	2.15	6 (19%)	40,43,43	1.67	10 (25%)
48	PLX	a	202	-	51,51,51	0.62	0	55,59,59	0.68	0
48	PLX	r	502	-	51,51,51	1.14	4 (7%)	55,59,59	0.62	1 (1%)
47	PEE	l	704	-	45,45,50	1.21	6 (13%)	48,50,55	1.03	2 (4%)
45	SF4	A	501	1	0,12,12	-	-	-		
53	CDL	l	702	-	99,99,99	1.09	8 (8%)	105,111,111	0.84	4 (3%)
55	UQ	s	401	-	28,28,63	3.29	7 (25%)	34,37,79	2.71	10 (29%)
45	SF4	M	801	12	0,12,12	-	-	-		
47	PEE	r	501	-	50,50,50	1.16	6 (12%)	53,55,55	1.01	2 (3%)
46	FMN	A	502	-	33,33,33	1.08	2 (6%)	48,50,50	1.23	8 (16%)
50	NDP	J	401	-	49,52,52	4.37	23 (46%)	66,80,80	2.20	12 (18%)
47	PEE	l	703	-	45,45,50	1.21	6 (13%)	48,50,55	0.99	2 (4%)
53	CDL	i	401	-	65,65,99	1.14	4 (6%)	71,77,111	1.19	5 (7%)
53	CDL	n	101	-	77,77,99	1.03	4 (5%)	83,89,111	1.10	4 (4%)
51	FES	M	803	12	0,4,4	-	-	-		
53	CDL	g	202	-	99,99,99	1.09	8 (8%)	105,111,111	0.85	4 (3%)
45	SF4	B	301	2	0,12,12	-	-	-		
53	CDL	l	701	-	98,98,99	1.09	8 (8%)	104,110,111	0.88	4 (3%)
53	CDL	a	201	-	90,90,99	0.96	4 (4%)	96,102,111	1.09	6 (6%)
51	FES	O	301	14	0,4,4	-	-	-		
47	PEE	U	101	-	50,50,50	1.14	6 (12%)	53,55,55	0.97	2 (3%)
47	PEE	B	303	-	50,50,50	1.16	6 (12%)	53,55,55	1.00	2 (3%)
47	PEE	m	201	-	40,40,50	1.16	5 (12%)	43,45,55	1.00	2 (4%)
48	PLX	j	202	-	51,51,51	1.15	4 (7%)	55,59,59	0.58	1 (1%)
45	SF4	M	802	12	0,12,12	-	-	-		
48	PLX	C	302	-	51,51,51	1.15	4 (7%)	55,59,59	0.61	1 (1%)
53	CDL	N	201	-	50,50,99	1.28	4 (8%)	56,62,111	1.31	6 (10%)
48	PLX	r	503	-	51,51,51	1.15	4 (7%)	55,59,59	0.60	1 (1%)
47	PEE	j	201	-	46,46,50	1.21	6 (13%)	49,51,55	0.98	2 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	PEE	i	402	-	-	19/50/50/54	-
45	SF4	C	301	3	-	-	0/6/5/5
45	SF4	B	302	2	-	-	0/6/5/5
48	PLX	g	201	-	-	21/55/55/55	-
49	8Q1	X	201	6	-	22/41/41/41	-
56	ADP	w	401	-	-	4/16/32/32	0/3/3/3
49	8Q1	G	201	6	-	15/41/41/41	-
48	PLX	a	202	-	-	18/55/55/55	-
48	PLX	r	502	-	-	21/55/55/55	-
47	PEE	l	704	-	-	26/49/49/54	-
45	SF4	A	501	1	-	-	0/6/5/5
53	CDL	l	702	-	-	62/110/110/110	-
55	UQ	s	401	-	-	9/21/45/87	0/1/1/1
45	SF4	M	801	12	-	-	0/6/5/5
47	PEE	r	501	-	-	22/54/54/54	-
46	FMN	A	502	-	-	5/18/18/18	0/3/3/3
50	NDP	J	401	-	-	9/34/77/77	0/4/5/5
47	PEE	l	703	-	-	26/49/49/54	-
53	CDL	i	401	-	-	26/76/76/110	-
53	CDL	n	101	-	-	32/88/88/110	-
51	FES	M	803	12	-	-	0/1/1/1
53	CDL	g	202	-	-	64/110/110/110	-
53	CDL	l	701	-	-	52/109/109/110	-
45	SF4	B	301	2	-	-	0/6/5/5
53	CDL	a	201	-	-	23/101/101/110	-
51	FES	O	301	14	-	-	0/1/1/1
47	PEE	U	101	-	-	23/54/54/54	-
47	PEE	B	303	-	-	23/54/54/54	-
47	PEE	m	201	-	-	22/44/44/54	-
48	PLX	j	202	-	-	31/55/55/55	-
45	SF4	M	802	12	-	-	0/6/5/5
48	PLX	C	302	-	-	29/55/55/55	-
53	CDL	N	201	-	-	23/61/61/110	-
48	PLX	r	503	-	-	32/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	PEE	j	201	-	-	23/50/50/54	-

All (159) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	J	401	NDP	C3B-C2B	-12.42	1.25	1.52
50	J	401	NDP	C6N-C5N	12.31	1.55	1.33
50	J	401	NDP	O4D-C4D	10.67	1.68	1.45
50	J	401	NDP	C3D-C4D	-9.92	1.27	1.53
55	s	401	UQ	C13-C14	9.35	1.55	1.33
56	w	401	ADP	C3'-C4'	-9.06	1.29	1.53
55	s	401	UQ	C8-C9	8.97	1.54	1.33
55	s	401	UQ	C18-C19	8.24	1.56	1.32
50	J	401	NDP	O4B-C4B	-7.97	1.27	1.45
49	X	201	8Q1	P24-O27	7.97	1.85	1.60
49	G	201	8Q1	P24-O27	7.81	1.85	1.60
56	w	401	ADP	O4'-C4'	7.74	1.62	1.45
50	J	401	NDP	C2N-C3N	7.39	1.55	1.34
50	J	401	NDP	C6A-N6A	5.90	1.48	1.34
50	J	401	NDP	P2B-O2B	5.61	1.69	1.59
56	w	401	ADP	C6-N6	5.55	1.48	1.34
50	J	401	NDP	C3B-C4B	5.36	1.66	1.53
50	J	401	NDP	O4D-C1D	-4.93	1.30	1.42
50	J	401	NDP	C6N-N1N	4.79	1.49	1.37
50	J	401	NDP	C1B-N9A	-4.56	1.33	1.46
50	J	401	NDP	O4B-C1B	4.49	1.52	1.42
53	N	201	CDL	OA8-CA7	4.31	1.45	1.33
53	a	201	CDL	OA8-CA7	4.29	1.45	1.33
53	i	401	CDL	OA8-CA7	4.27	1.45	1.33
53	n	101	CDL	OA8-CA7	4.27	1.45	1.33
53	i	401	CDL	OB8-CB7	4.26	1.45	1.33
53	N	201	CDL	OB8-CB7	4.25	1.45	1.33
56	w	401	ADP	O4'-C1'	-4.25	1.31	1.42
50	J	401	NDP	O2D-C2D	-4.22	1.33	1.43
50	J	401	NDP	C7N-N7N	4.21	1.44	1.33
53	n	101	CDL	OB8-CB7	4.20	1.45	1.33
49	G	201	8Q1	C1-S44	4.17	1.86	1.76
53	i	401	CDL	OA6-CA5	4.17	1.46	1.34
53	i	401	CDL	OB6-CB5	4.16	1.46	1.34
53	n	101	CDL	OA6-CA5	4.15	1.46	1.34
53	a	201	CDL	OB8-CB7	4.15	1.45	1.33
53	a	201	CDL	OA6-CA5	4.14	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	N	201	CDL	OA6-CA5	4.13	1.45	1.34
53	a	201	CDL	OB6-CB5	4.09	1.45	1.34
53	N	201	CDL	OB6-CB5	4.07	1.45	1.34
53	n	101	CDL	OB6-CB5	3.95	1.45	1.34
46	A	502	FMN	C4A-N5	3.91	1.38	1.30
49	X	201	8Q1	C1-S44	3.89	1.85	1.76
47	m	201	PEE	C18-C19	3.76	1.53	1.31
47	j	201	PEE	C18-C19	3.75	1.53	1.31
47	l	703	PEE	C18-C19	3.72	1.53	1.31
47	l	704	PEE	C18-C19	3.71	1.53	1.31
47	B	303	PEE	C18-C19	3.71	1.53	1.31
47	r	501	PEE	C18-C19	3.71	1.53	1.31
47	U	101	PEE	C18-C19	3.68	1.53	1.31
47	i	402	PEE	C18-C19	3.67	1.53	1.31
47	j	201	PEE	C39-C38	3.65	1.52	1.31
49	G	201	8Q1	C34-N36	3.65	1.41	1.33
49	X	201	8Q1	C34-N36	3.63	1.41	1.33
47	r	501	PEE	C39-C38	3.63	1.52	1.31
47	B	303	PEE	C39-C38	3.62	1.52	1.31
47	i	402	PEE	C39-C38	3.62	1.52	1.31
47	l	703	PEE	C39-C38	3.62	1.52	1.31
47	U	101	PEE	C39-C38	3.62	1.52	1.31
47	l	704	PEE	C39-C38	3.61	1.52	1.31
49	X	201	8Q1	C6-C1	3.52	1.54	1.50
53	l	701	CDL	OA8-CA7	3.46	1.43	1.33
53	l	702	CDL	OA8-CA7	3.45	1.43	1.33
53	g	202	CDL	OA8-CA7	3.43	1.43	1.33
49	G	201	8Q1	C6-C1	3.37	1.54	1.50
56	w	401	ADP	O2'-C2'	-3.33	1.35	1.43
49	G	201	8Q1	O27-C28	-3.25	1.33	1.43
49	X	201	8Q1	O27-C28	-3.22	1.33	1.43
49	X	201	8Q1	C39-N41	3.21	1.40	1.33
49	G	201	8Q1	C39-N41	3.19	1.40	1.33
56	w	401	ADP	O3'-C3'	3.13	1.50	1.43
56	w	401	ADP	C8-N9	-3.12	1.31	1.37
50	J	401	NDP	C8A-N9A	-3.09	1.32	1.37
53	l	702	CDL	OB6-CB5	3.07	1.43	1.34
53	l	701	CDL	OB6-CB5	3.05	1.42	1.34
50	J	401	NDP	O3D-C3D	3.05	1.50	1.43
53	g	202	CDL	OB6-CB5	3.05	1.42	1.34
50	J	401	NDP	C5A-N7A	-3.03	1.33	1.39
53	l	701	CDL	OB8-CB7	3.00	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	l	702	CDL	OB8-CB7	3.00	1.42	1.33
53	g	202	CDL	OB8-CB7	2.99	1.42	1.33
53	g	202	CDL	OA6-CA5	2.98	1.42	1.34
53	l	702	CDL	OA6-CA5	2.97	1.42	1.34
50	J	401	NDP	C7N-C3N	2.96	1.55	1.48
53	l	701	CDL	OA6-CA5	2.91	1.42	1.34
48	g	201	PLX	O6-C4	-2.71	1.41	1.44
48	C	302	PLX	O6-C4	-2.66	1.41	1.44
48	r	503	PLX	O6-C4	-2.65	1.41	1.44
48	j	202	PLX	O6-C4	-2.65	1.41	1.44
55	s	401	UQ	C6-C1	2.63	1.54	1.46
50	J	401	NDP	O2B-C2B	2.58	1.53	1.44
47	i	402	PEE	O3-C30	2.52	1.40	1.33
47	r	501	PEE	O2-C2	-2.49	1.40	1.46
47	r	501	PEE	O3-C30	2.48	1.40	1.33
47	B	303	PEE	O2-C2	-2.48	1.40	1.46
47	l	703	PEE	O2-C2	-2.47	1.40	1.46
46	A	502	FMN	C10-N1	2.46	1.38	1.33
47	j	201	PEE	O2-C2	-2.46	1.40	1.46
47	i	402	PEE	O2-C2	-2.46	1.40	1.46
47	B	303	PEE	O3-C30	2.46	1.40	1.33
47	l	704	PEE	O2-C2	-2.46	1.40	1.46
47	l	703	PEE	O3-C30	2.44	1.40	1.33
48	j	202	PLX	C7-C6	2.42	1.55	1.50
53	l	701	CDL	OA6-CA4	-2.41	1.40	1.46
47	j	201	PEE	O3-C30	2.41	1.40	1.33
47	l	704	PEE	O3-C30	2.40	1.40	1.33
53	l	702	CDL	OA6-CA4	-2.40	1.40	1.46
47	m	201	PEE	O2-C10	2.39	1.41	1.34
47	U	101	PEE	O3-C30	2.39	1.40	1.33
48	g	201	PLX	C7-C6	2.37	1.55	1.50
53	g	202	CDL	OA6-CA4	-2.37	1.40	1.46
48	r	502	PLX	C7-C6	2.34	1.55	1.50
47	U	101	PEE	O2-C2	-2.34	1.40	1.46
55	s	401	UQ	C7-C8	2.33	1.54	1.50
50	J	401	NDP	C2D-C3D	2.32	1.59	1.53
48	C	302	PLX	C7-C6	2.31	1.55	1.50
47	U	101	PEE	O2-C10	2.30	1.40	1.34
48	r	503	PLX	C7-C6	2.29	1.55	1.50
47	j	201	PEE	O2-C10	2.29	1.40	1.34
47	m	201	PEE	O3-C30	2.29	1.40	1.33
56	w	401	ADP	C5-N7	-2.28	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	i	402	PEE	O2-C10	2.26	1.40	1.34
48	r	502	PLX	O6-C4	-2.24	1.41	1.44
47	m	201	PEE	O2-C2	-2.23	1.41	1.46
53	g	202	CDL	PB2-OB2	2.23	1.68	1.59
47	m	201	PEE	O3-C3	-2.22	1.40	1.45
53	l	701	CDL	PB2-OB2	2.22	1.68	1.59
53	l	702	CDL	PB2-OB2	2.21	1.68	1.59
53	g	202	CDL	PB2-OB5	2.20	1.68	1.59
47	l	704	PEE	O3-C3	-2.20	1.40	1.45
47	r	501	PEE	O2-C10	2.19	1.40	1.34
53	l	702	CDL	PB2-OB5	2.19	1.68	1.59
47	B	303	PEE	O2-C10	2.18	1.40	1.34
53	l	701	CDL	PB2-OB5	2.17	1.68	1.59
47	l	704	PEE	O2-C10	2.17	1.40	1.34
55	s	401	UQ	O4-C4	-2.17	1.18	1.23
47	l	703	PEE	O3-C3	-2.16	1.40	1.45
50	J	401	NDP	O7N-C7N	-2.16	1.19	1.24
48	j	202	PLX	P1-O4	2.15	1.68	1.59
48	r	502	PLX	P1-O4	2.14	1.68	1.59
48	r	503	PLX	P1-O4	2.14	1.68	1.59
47	l	703	PEE	O2-C10	2.14	1.40	1.34
47	j	201	PEE	O3-C3	-2.13	1.40	1.45
53	l	701	CDL	OB6-CB4	-2.13	1.41	1.46
48	C	302	PLX	P1-O4	2.12	1.67	1.59
47	i	402	PEE	O3-C3	-2.12	1.40	1.45
55	s	401	UQ	O1-C1	-2.11	1.18	1.23
53	l	702	CDL	OB6-CB4	-2.11	1.41	1.46
48	g	201	PLX	P1-O4	2.11	1.67	1.59
53	g	202	CDL	OB6-CB4	-2.11	1.41	1.46
47	U	101	PEE	O3-C3	-2.09	1.40	1.45
47	r	501	PEE	O3-C3	-2.07	1.40	1.45
48	C	302	PLX	P1-O1	2.05	1.67	1.59
48	r	503	PLX	P1-O1	2.05	1.67	1.59
48	r	502	PLX	P1-O1	2.04	1.67	1.59
47	B	303	PEE	O3-C3	-2.04	1.40	1.45
48	j	202	PLX	P1-O1	2.03	1.67	1.59
48	g	201	PLX	P1-O1	2.01	1.67	1.59
50	J	401	NDP	PA-O5B	2.00	1.67	1.59

All (112) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	s	401	UQ	C7-C8-C9	-9.04	111.75	126.79
50	J	401	NDP	C3N-C2N-N1N	-8.29	111.27	123.10
50	J	401	NDP	C1D-N1N-C2N	-6.58	110.16	121.11
50	J	401	NDP	C5A-C4A-N3A	-5.90	119.06	126.75
55	s	401	UQ	C12-C13-C14	-5.87	113.52	127.66
56	w	401	ADP	C5-C4-N3	-5.75	119.25	126.75
50	J	401	NDP	C1D-N1N-C6N	-4.90	110.28	120.83
49	X	201	8Q1	C6-C1-S44	4.67	118.89	113.46
55	s	401	UQ	C11-C9-C8	-4.55	111.91	121.12
56	w	401	ADP	N3-C4-N9	4.45	134.42	127.08
55	s	401	UQ	C10-C9-C8	-4.43	112.32	123.68
56	w	401	ADP	N3-C2-N1	-4.39	121.73	128.60
49	G	201	8Q1	C6-C1-S44	4.33	118.49	113.46
53	i	401	CDL	OA6-CA5-C11	4.32	120.80	111.50
47	B	303	PEE	O2-C10-C11	4.31	120.80	111.50
53	a	201	CDL	OB6-CB5-C51	4.26	120.68	111.50
50	J	401	NDP	N3A-C4A-N9A	4.24	134.06	127.08
47	r	501	PEE	O2-C10-C11	4.19	120.52	111.50
47	m	201	PEE	O2-C10-C11	4.17	120.50	111.50
55	s	401	UQ	C15-C14-C13	-4.14	113.06	123.68
53	N	201	CDL	OB6-CB5-C51	4.12	120.38	111.50
50	J	401	NDP	N3A-C2A-N1A	-4.12	122.16	128.60
53	n	101	CDL	OA6-CA5-C11	4.10	120.35	111.50
47	i	402	PEE	O2-C10-C11	4.10	120.33	111.50
53	N	201	CDL	OA6-CA5-C11	4.07	120.28	111.50
55	s	401	UQ	C17-C18-C19	-4.03	113.98	127.75
55	s	401	UQ	C16-C14-C13	-4.01	113.01	121.12
47	l	704	PEE	O2-C10-C11	4.00	120.12	111.50
47	j	201	PEE	O2-C10-C11	3.98	120.08	111.50
53	g	202	CDL	OB6-CB5-C51	3.98	120.08	111.50
53	l	701	CDL	OA6-CA5-C11	3.95	120.02	111.50
53	i	401	CDL	OB6-CB5-C51	3.95	120.02	111.50
53	l	702	CDL	OB6-CB5-C51	3.95	120.02	111.50
53	l	701	CDL	OB6-CB5-C51	3.93	119.97	111.50
47	U	101	PEE	O2-C10-C11	3.92	119.94	111.50
53	g	202	CDL	OA6-CA5-C11	3.91	119.93	111.50
53	n	101	CDL	OB6-CB5-C51	3.89	119.89	111.50
53	l	702	CDL	OA6-CA5-C11	3.89	119.88	111.50
47	l	703	PEE	O2-C10-C11	3.86	119.81	111.50
50	J	401	NDP	C2A-N3A-C4A	3.80	120.72	111.75
56	w	401	ADP	C2-N3-C4	3.71	120.52	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	401	ADP	N9-C8-N7	-3.66	108.91	113.91
49	G	201	8Q1	C43-S44-C1	3.58	113.03	101.87
53	a	201	CDL	OA6-CA5-C11	3.53	119.10	111.50
56	w	401	ADP	C5-N7-C8	3.49	108.46	103.51
55	s	401	UQ	C21-C19-C18	-3.33	113.03	122.65
49	G	201	8Q1	O35-C34-N36	-3.28	115.96	122.99
49	X	201	8Q1	C43-S44-C1	3.26	112.01	101.87
50	J	401	NDP	N9A-C8A-N7A	-3.24	109.48	113.91
50	J	401	NDP	C5A-N7A-C8A	3.23	108.10	103.51
49	X	201	8Q1	O35-C34-N36	-3.20	116.13	122.99
56	w	401	ADP	C4-N9-C8	3.12	109.11	105.73
46	A	502	FMN	C4-N3-C2	-3.09	119.93	125.64
55	s	401	UQ	C20-C19-C18	-3.08	113.73	122.65
53	a	201	CDL	OB8-CB7-C71	2.92	121.08	111.91
53	a	201	CDL	OA8-CA7-C31	2.92	121.06	111.91
49	G	201	8Q1	C37-C38-C39	2.90	117.18	112.36
55	s	401	UQ	CM5-C5-C6	-2.87	119.72	124.40
53	i	401	CDL	OA8-CA7-C31	2.87	120.90	111.91
50	J	401	NDP	PN-O3-PA	-2.86	123.02	132.83
50	J	401	NDP	C4A-C5A-N7A	-2.85	107.15	110.62
56	w	401	ADP	C4-C5-N7	-2.81	107.19	110.62
49	X	201	8Q1	O2-P24-O27	-2.80	99.27	106.73
47	l	703	PEE	O3-C30-C31	2.80	120.68	111.91
49	G	201	8Q1	O2-P24-O27	-2.79	99.32	106.73
53	N	201	CDL	OA8-CA7-C31	2.79	120.65	111.91
47	r	501	PEE	O3-C30-C31	2.77	120.61	111.91
47	B	303	PEE	O3-C30-C31	2.74	120.52	111.91
53	n	101	CDL	OA8-CA7-C31	2.74	120.50	111.91
53	a	201	CDL	CB4-OB6-CB5	-2.74	111.05	117.79
56	w	401	ADP	PA-O3A-PB	-2.72	123.48	132.83
47	l	704	PEE	O3-C30-C31	2.69	120.33	111.91
46	A	502	FMN	C4A-C4-N3	2.66	119.95	113.19
53	N	201	CDL	OB8-CB7-C71	2.66	120.25	111.91
53	l	701	CDL	OB8-CB7-C71	2.63	120.16	111.91
49	X	201	8Q1	C37-C38-C39	2.60	116.68	112.36
53	l	702	CDL	OA8-CA7-C31	2.59	120.04	111.91
53	n	101	CDL	OB8-CB7-C71	2.59	120.03	111.91
53	g	202	CDL	OB8-CB7-C71	2.58	120.02	111.91
53	l	701	CDL	OA8-CA7-C31	2.58	120.00	111.91
47	U	101	PEE	O3-C30-C31	2.57	119.97	111.91
47	m	201	PEE	O3-C30-C31	2.56	119.93	111.91
53	N	201	CDL	CB4-OB6-CB5	-2.56	111.50	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	l	702	CDL	OB8-CB7-C71	2.54	119.88	111.91
47	i	402	PEE	O3-C30-C31	2.53	119.86	111.91
47	j	201	PEE	O3-C30-C31	2.50	119.77	111.91
53	g	202	CDL	OA8-CA7-C31	2.49	119.72	111.91
48	r	503	PLX	C1A-N1-C1	2.48	120.07	109.92
49	X	201	8Q1	C32-C34-N36	2.47	121.50	116.58
46	A	502	FMN	O4-C4-C4A	-2.46	120.07	126.60
50	J	401	NDP	C4A-N9A-C8A	2.46	108.39	105.73
49	X	201	8Q1	O4-C1-S44	-2.46	119.42	122.61
46	A	502	FMN	C4A-C10-N10	2.44	120.04	116.48
48	r	502	PLX	C1A-N1-C1	2.42	119.81	109.92
48	j	202	PLX	C1A-N1-C1	2.41	119.79	109.92
53	i	401	CDL	OB8-CB7-C71	2.41	119.47	111.91
49	G	201	8Q1	O40-C39-N41	-2.41	118.47	123.01
49	G	201	8Q1	O1-P24-O2	2.39	116.78	107.64
49	X	201	8Q1	O1-P24-O2	2.38	116.72	107.64
49	G	201	8Q1	C32-C34-N36	2.37	121.30	116.58
48	g	201	PLX	C1A-N1-C1	2.34	119.50	109.92
46	A	502	FMN	C10-C4A-N5	-2.24	120.10	124.86
49	X	201	8Q1	O40-C39-N41	-2.23	118.80	123.01
46	A	502	FMN	C4A-C10-N1	-2.23	119.56	124.73
46	A	502	FMN	C9A-C5A-N5	-2.22	120.02	122.43
48	C	302	PLX	C1A-N1-C1	2.21	118.95	109.92
46	A	502	FMN	C5A-C9A-N10	2.11	120.14	117.95
49	G	201	8Q1	O4-C1-C6	-2.07	121.54	123.99
53	a	201	CDL	OB8-CB7-OB9	-2.04	118.44	123.59
49	G	201	8Q1	O4-C1-S44	-2.04	119.96	122.61
53	i	401	CDL	CA4-OA6-CA5	-2.04	112.77	117.79
53	N	201	CDL	CA6-CA4-CA3	-2.02	107.01	111.79

There are no chirality outliers.

All (682) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
46	A	502	FMN	C3'-C4'-C5'-O5'
47	U	101	PEE	C19-C20-C21-C22
47	U	101	PEE	C4-O4P-P-O3P
47	U	101	PEE	C4-O4P-P-O2P
47	U	101	PEE	C4-O4P-P-O1P
47	i	402	PEE	C11-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
47	j	201	PEE	C1-O3P-P-O2P
47	j	201	PEE	C1-O3P-P-O1P
47	l	703	PEE	C11-C10-O2-C2
47	l	703	PEE	C4-O4P-P-O2P
47	l	703	PEE	C4-O4P-P-O1P
47	m	201	PEE	C11-C10-O2-C2
47	m	201	PEE	C3-C2-O2-C10
47	r	501	PEE	C15-C16-C17-C18
48	C	302	PLX	C3-O4-P1-O2
48	C	302	PLX	C3-O4-P1-O3
48	C	302	PLX	N1-C1-C2-O1
48	a	202	PLX	C3-O4-P1-O1
48	a	202	PLX	C3-O4-P1-O2
48	a	202	PLX	C3-O4-P1-O3
48	a	202	PLX	O9-C24-O8-C5
48	a	202	PLX	O9-C24-C25-C26
48	g	201	PLX	O7-C6-O6-C4
48	j	202	PLX	O7-C6-C7-C8
48	j	202	PLX	O7-C6-O6-C4
48	j	202	PLX	O9-C24-O8-C5
48	r	502	PLX	O7-C6-O6-C4
48	r	502	PLX	C5-C4-O6-C6
48	r	503	PLX	C3-O4-P1-O1
48	r	503	PLX	C2-O1-P1-O4
48	r	503	PLX	C2-O1-P1-O2
48	r	503	PLX	C2-O1-P1-O3
48	r	503	PLX	C25-C24-O8-C5
48	r	503	PLX	O9-C24-C25-C26
49	G	201	8Q1	O4-C1-S44-C43
49	G	201	8Q1	C6-C1-S44-C43
49	G	201	8Q1	O27-C28-C29-C31
49	G	201	8Q1	O27-C28-C29-C32
49	G	201	8Q1	C42-C43-S44-C1
49	X	201	8Q1	C1-C6-C7-C8
49	X	201	8Q1	C28-C29-C32-C34
49	X	201	8Q1	C28-C29-C32-O33
49	X	201	8Q1	C30-C29-C32-C34
49	X	201	8Q1	C30-C29-C32-O33
49	X	201	8Q1	C31-C29-C32-C34
49	X	201	8Q1	N36-C37-C38-C39
49	X	201	8Q1	C42-C43-S44-C1
49	X	201	8Q1	C28-O27-P24-O2

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Mol	Chain	Res	Type	Atoms
50	J	401	NDP	C5B-O5B-PA-O1A
50	J	401	NDP	C2B-O2B-P2B-O1X
53	N	201	CDL	O1-C1-CB2-OB2
53	N	201	CDL	CA2-C1-CB2-OB2
53	N	201	CDL	CA2-OA2-PA1-OA3
53	N	201	CDL	CA2-OA2-PA1-OA4
53	N	201	CDL	CA2-OA2-PA1-OA5
53	N	201	CDL	CA3-OA5-PA1-OA4
53	N	201	CDL	CA6-CA4-OA6-CA5
53	N	201	CDL	CB2-OB2-PB2-OB4
53	N	201	CDL	CB3-OB5-PB2-OB2
53	a	201	CDL	CA2-OA2-PA1-OA3
53	a	201	CDL	CB2-OB2-PB2-OB3
53	a	201	CDL	CB3-OB5-PB2-OB3
53	g	202	CDL	CA2-OA2-PA1-OA3
53	g	202	CDL	CA2-OA2-PA1-OA4
53	g	202	CDL	CA3-OA5-PA1-OA2
53	g	202	CDL	CA3-OA5-PA1-OA3
53	g	202	CDL	CA3-OA5-PA1-OA4
53	g	202	CDL	CB2-OB2-PB2-OB3
53	g	202	CDL	CB2-OB2-PB2-OB5
53	i	401	CDL	CB2-C1-CA2-OA2
53	i	401	CDL	O1-C1-CB2-OB2
53	i	401	CDL	CA2-OA2-PA1-OA4
53	i	401	CDL	CA3-OA5-PA1-OA2
53	i	401	CDL	CB3-OB5-PB2-OB3
53	i	401	CDL	OB6-CB4-CB6-OB8
53	l	701	CDL	O1-C1-CA2-OA2
53	l	701	CDL	O1-C1-CB2-OB2
53	l	701	CDL	CA2-OA2-PA1-OA3
53	l	701	CDL	CA2-OA2-PA1-OA4
53	l	701	CDL	CA2-OA2-PA1-OA5
53	l	701	CDL	CA3-OA5-PA1-OA3
53	l	701	CDL	CB2-OB2-PB2-OB3
53	l	701	CDL	CB2-OB2-PB2-OB4
53	l	701	CDL	CB2-OB2-PB2-OB5
53	l	702	CDL	O1-C1-CA2-OA2
53	l	702	CDL	O1-C1-CB2-OB2
53	l	702	CDL	CA3-OA5-PA1-OA2
53	l	702	CDL	CA3-OA5-PA1-OA3
53	l	702	CDL	CA3-OA5-PA1-OA4
53	l	702	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
53	l	702	CDL	CB2-OB2-PB2-OB3
53	l	702	CDL	OB6-CB4-CB6-OB8
53	n	101	CDL	CA2-OA2-PA1-OA3
53	n	101	CDL	CA2-OA2-PA1-OA4
53	n	101	CDL	CA2-OA2-PA1-OA5
53	n	101	CDL	CA3-OA5-PA1-OA2
53	n	101	CDL	CA3-OA5-PA1-OA3
53	n	101	CDL	CA3-OA5-PA1-OA4
53	n	101	CDL	CB2-OB2-PB2-OB4
53	n	101	CDL	CB3-OB5-PB2-OB3
55	s	401	UQ	C7-C8-C9-C11
55	s	401	UQ	C12-C11-C9-C10
55	s	401	UQ	C12-C13-C14-C16
56	w	401	ADP	C5'-O5'-PA-O1A
56	w	401	ADP	C5'-O5'-PA-O2A
56	w	401	ADP	C5'-O5'-PA-O3A
53	l	701	CDL	OA9-CA7-OA8-CA6
53	l	701	CDL	C31-CA7-OA8-CA6
47	i	402	PEE	O4-C10-O2-C2
47	m	201	PEE	O4-C10-O2-C2
47	r	501	PEE	O4-C10-O2-C2
53	N	201	CDL	OA7-CA5-OA6-CA4
53	g	202	CDL	C71-CB7-OB8-CB6
47	r	501	PEE	C11-C10-O2-C2
53	N	201	CDL	C11-CA5-OA6-CA4
47	B	303	PEE	C17-C18-C19-C20
47	B	303	PEE	C37-C38-C39-C40
47	U	101	PEE	C17-C18-C19-C20
55	s	401	UQ	C17-C18-C19-C21
55	s	401	UQ	C7-C8-C9-C10
47	l	703	PEE	O4-C10-O2-C2
53	l	702	CDL	OB9-CB7-OB8-CB6
47	U	101	PEE	C31-C30-O3-C3
53	l	702	CDL	C71-CB7-OB8-CB6
53	g	202	CDL	OB9-CB7-OB8-CB6
47	B	303	PEE	C11-C10-O2-C2
47	U	101	PEE	C11-C10-O2-C2
47	j	201	PEE	C11-C10-O2-C2
53	g	202	CDL	C51-CB5-OB6-CB4
48	r	503	PLX	C12-C13-C14-C15
48	C	302	PLX	C28-C29-C30-C31
48	r	502	PLX	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
47	U	101	PEE	C30-C31-C32-C33
53	l	702	CDL	C11-C12-C13-C14
53	l	702	CDL	C35-C36-C37-C38
47	U	101	PEE	O5-C30-O3-C3
55	s	401	UQ	C9-C11-C12-C13
48	j	202	PLX	C28-C29-C30-C31
47	m	201	PEE	C31-C30-O3-C3
53	l	701	CDL	C55-C56-C57-C58
48	g	201	PLX	C12-C13-C14-C15
53	g	202	CDL	CB2-C1-CA2-OA2
53	i	401	CDL	CA2-C1-CB2-OB2
53	l	701	CDL	CA2-C1-CB2-OB2
53	l	702	CDL	CA2-C1-CB2-OB2
47	j	201	PEE	O4-C10-O2-C2
48	r	503	PLX	C2-C1-N1-C1A
53	i	401	CDL	C31-CA7-OA8-CA6
47	l	704	PEE	C10-C11-C12-C13
47	m	201	PEE	C33-C34-C35-C36
53	N	201	CDL	O1-C1-CA2-OA2
53	i	401	CDL	O1-C1-CA2-OA2
47	l	703	PEE	C31-C30-O3-C3
53	a	201	CDL	C31-C32-C33-C34
47	m	201	PEE	O5-C30-O3-C3
53	i	401	CDL	OA9-CA7-OA8-CA6
47	U	101	PEE	O4-C10-O2-C2
53	n	101	CDL	C11-CA5-OA6-CA4
47	i	402	PEE	C10-C11-C12-C13
47	r	501	PEE	C10-C11-C12-C13
53	l	701	CDL	CB7-C71-C72-C73
50	J	401	NDP	C2D-C1D-N1N-C6N
53	l	702	CDL	C59-C60-C61-C62
48	j	202	PLX	C15-C16-C17-C18
53	l	702	CDL	CB5-C51-C52-C53
47	r	501	PEE	C17-C18-C19-C20
47	r	501	PEE	C30-C31-C32-C33
53	l	702	CDL	CB7-C71-C72-C73
53	n	101	CDL	C75-C76-C77-C78
50	J	401	NDP	O4B-C4B-C5B-O5B
47	B	303	PEE	O4-C10-O2-C2
53	g	202	CDL	OB7-CB5-OB6-CB4
48	g	201	PLX	C7-C8-C9-C10
48	r	503	PLX	C2-C1-N1-C1C

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Mol	Chain	Res	Type	Atoms
53	g	202	CDL	CA7-C31-C32-C33
53	N	201	CDL	C51-CB5-OB6-CB4
47	l	703	PEE	O5-C30-O3-C3
48	r	502	PLX	C30-C31-C32-C33
47	i	402	PEE	C22-C23-C24-C25
53	g	202	CDL	O1-C1-CA2-OA2
53	l	702	CDL	C54-C55-C56-C57
47	j	201	PEE	C1-O3P-P-O4P
47	l	703	PEE	C4-O4P-P-O3P
47	l	704	PEE	C1-O3P-P-O4P
47	m	201	PEE	C4-O4P-P-O3P
47	r	501	PEE	C1-O3P-P-O4P
48	C	302	PLX	C3-O4-P1-O1
48	j	202	PLX	C3-O4-P1-O1
53	N	201	CDL	CA3-OA5-PA1-OA2
53	N	201	CDL	CB2-OB2-PB2-OB5
53	a	201	CDL	CA2-OA2-PA1-OA5
53	a	201	CDL	CB2-OB2-PB2-OB5
53	g	202	CDL	CA2-OA2-PA1-OA5
53	g	202	CDL	CB3-OB5-PB2-OB2
53	i	401	CDL	CA2-OA2-PA1-OA5
53	i	401	CDL	CB2-OB2-PB2-OB5
53	l	702	CDL	CB2-OB2-PB2-OB5
53	l	702	CDL	CB3-OB5-PB2-OB2
53	n	101	CDL	CB2-OB2-PB2-OB5
53	l	701	CDL	CB2-C1-CA2-OA2
53	l	702	CDL	CB2-C1-CA2-OA2
53	N	201	CDL	OB7-CB5-OB6-CB4
53	n	101	CDL	OA7-CA5-OA6-CA4
47	l	704	PEE	C31-C30-O3-C3
48	C	302	PLX	O8-C24-C25-C26
48	j	202	PLX	O6-C6-C7-C8
53	a	201	CDL	C39-C40-C41-C42
48	C	302	PLX	C25-C26-C27-C28
48	g	201	PLX	C33-C34-C35-C36
53	l	701	CDL	C52-C53-C54-C55
47	r	501	PEE	C13-C14-C15-C16
48	r	502	PLX	C27-C28-C29-C30
53	l	701	CDL	C74-C75-C76-C77
53	l	702	CDL	C33-C34-C35-C36
53	l	702	CDL	C55-C56-C57-C58
53	l	702	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
53	l	702	CDL	C73-C74-C75-C76
49	G	201	8Q1	O27-C28-C29-C30
47	B	303	PEE	C22-C23-C24-C25
48	g	201	PLX	C9-C10-C11-C12
48	j	202	PLX	C25-C26-C27-C28
48	r	502	PLX	C33-C34-C35-C36
48	r	503	PLX	C25-C26-C27-C28
49	G	201	8Q1	C11-C12-C13-C14
53	g	202	CDL	C71-C72-C73-C74
53	l	701	CDL	C82-C83-C84-C85
53	l	702	CDL	C37-C38-C39-C40
53	l	702	CDL	C58-C59-C60-C61
53	l	702	CDL	C63-C64-C65-C66
53	n	101	CDL	CA6-CA4-OA6-CA5
47	l	703	PEE	C21-C22-C23-C24
47	r	501	PEE	C12-C13-C14-C15
49	X	201	8Q1	C11-C12-C13-C14
53	l	701	CDL	C62-C63-C64-C65
47	l	704	PEE	C17-C18-C19-C20
47	l	704	PEE	C33-C34-C35-C36
48	C	302	PLX	C14-C15-C16-C17
48	j	202	PLX	C27-C28-C29-C30
48	g	201	PLX	C25-C26-C27-C28
48	r	502	PLX	C7-C8-C9-C10
53	l	701	CDL	C35-C36-C37-C38
53	l	701	CDL	C56-C57-C58-C59
53	g	202	CDL	CB5-C51-C52-C53
47	j	201	PEE	C42-C43-C44-C45
48	r	503	PLX	C28-C29-C30-C31
53	g	202	CDL	C56-C57-C58-C59
53	g	202	CDL	C59-C60-C61-C62
47	l	703	PEE	C23-C24-C25-C26
48	g	201	PLX	C11-C10-C9-C8
48	r	503	PLX	C13-C14-C15-C16
53	g	202	CDL	C73-C74-C75-C76
48	j	202	PLX	C7-C8-C9-C10
48	r	502	PLX	C10-C11-C12-C13
48	r	503	PLX	C14-C15-C16-C17
48	r	503	PLX	C29-C30-C31-C32
53	g	202	CDL	C12-C13-C14-C15
53	g	202	CDL	C14-C15-C16-C17
53	g	202	CDL	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
47	U	101	PEE	C22-C23-C24-C25
47	l	704	PEE	C34-C35-C36-C37
48	C	302	PLX	C18-C19-C20-C21
49	G	201	8Q1	C6-C7-C8-C9
53	g	202	CDL	C75-C76-C77-C78
53	l	701	CDL	C75-C76-C77-C78
47	l	704	PEE	C11-C10-O2-C2
48	C	302	PLX	C16-C17-C18-C19
48	r	503	PLX	C33-C34-C35-C36
49	G	201	8Q1	C12-C13-C14-C15
53	l	701	CDL	C20-C21-C22-C23
49	G	201	8Q1	C10-C11-C12-C13
53	g	202	CDL	C33-C34-C35-C36
53	g	202	CDL	C35-C36-C37-C38
53	i	401	CDL	C36-C37-C38-C39
53	l	701	CDL	C14-C15-C16-C17
53	l	701	CDL	C73-C74-C75-C76
47	r	501	PEE	C41-C42-C43-C44
48	C	302	PLX	C17-C18-C19-C20
48	C	302	PLX	C9-C10-C11-C12
48	r	502	PLX	C14-C15-C16-C17
53	g	202	CDL	C52-C53-C54-C55
48	g	201	PLX	C31-C32-C33-C34
53	i	401	CDL	C33-C34-C35-C36
47	m	201	PEE	C11-C12-C13-C14
48	g	201	PLX	C10-C11-C12-C13
46	A	502	FMN	O4'-C4'-C5'-O5'
53	g	202	CDL	CB7-C71-C72-C73
48	r	503	PLX	C10-C11-C12-C13
53	g	202	CDL	C43-C44-C45-C46
53	l	701	CDL	C11-C12-C13-C14
47	l	704	PEE	O5-C30-O3-C3
53	a	201	CDL	C51-CB5-OB6-CB4
48	C	302	PLX	O9-C24-C25-C26
48	j	202	PLX	C10-C11-C12-C13
53	g	202	CDL	C62-C63-C64-C65
53	i	401	CDL	C11-C12-C13-C14
53	l	701	CDL	C32-C33-C34-C35
47	B	303	PEE	C30-C31-C32-C33
48	C	302	PLX	C33-C34-C35-C36
53	l	701	CDL	C61-C62-C63-C64
47	l	704	PEE	O4-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
53	a	201	CDL	OB7-CB5-OB6-CB4
48	j	202	PLX	C12-C13-C14-C15
47	B	303	PEE	C14-C15-C16-C17
53	a	201	CDL	C73-C74-C75-C76
48	j	202	PLX	C2-C1-N1-C1A
48	r	503	PLX	C2-C1-N1-C1B
53	l	702	CDL	C39-C40-C41-C42
47	B	303	PEE	C20-C21-C22-C23
48	j	202	PLX	C13-C14-C15-C16
53	l	702	CDL	C40-C41-C42-C43
47	l	703	PEE	C37-C38-C39-C40
53	g	202	CDL	C41-C42-C43-C44
53	n	101	CDL	C53-C54-C55-C56
47	i	402	PEE	C35-C36-C37-C38
47	l	703	PEE	C19-C20-C21-C22
47	l	703	PEE	C30-C31-C32-C33
47	B	303	PEE	C13-C14-C15-C16
47	l	703	PEE	C31-C32-C33-C34
48	r	502	PLX	C28-C29-C30-C31
48	C	302	PLX	C15-C16-C17-C18
49	G	201	8Q1	N36-C37-C38-C39
47	U	101	PEE	C42-C43-C44-C45
48	C	302	PLX	C26-C27-C28-C29
48	C	302	PLX	C30-C31-C32-C33
53	a	201	CDL	C18-C19-C20-C21
53	g	202	CDL	C17-C18-C19-C20
53	g	202	CDL	OB6-CB4-CB6-OB8
47	j	201	PEE	C20-C21-C22-C23
48	j	202	PLX	C26-C27-C28-C29
47	j	201	PEE	C11-C12-C13-C14
48	C	302	PLX	C27-C28-C29-C30
53	g	202	CDL	C82-C83-C84-C85
47	j	201	PEE	C15-C16-C17-C18
47	m	201	PEE	C19-C20-C21-C22
47	r	501	PEE	C39-C40-C41-C42
55	s	401	UQ	C12-C11-C9-C8
47	U	101	PEE	C32-C33-C34-C35
53	g	202	CDL	C61-C62-C63-C64
53	n	101	CDL	C58-C59-C60-C61
47	j	201	PEE	C34-C35-C36-C37
53	l	701	CDL	C51-C52-C53-C54
53	l	701	CDL	C60-C61-C62-C63

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Mol	Chain	Res	Type	Atoms
47	i	402	PEE	C14-C15-C16-C17
53	l	701	CDL	C58-C59-C60-C61
47	U	101	PEE	C36-C37-C38-C39
47	l	704	PEE	C18-C19-C20-C21
47	r	501	PEE	C36-C37-C38-C39
53	n	101	CDL	CB3-OB5-PB2-OB2
48	C	302	PLX	C7-C8-C9-C10
48	a	202	PLX	C25-C26-C27-C28
53	l	701	CDL	C71-C72-C73-C74
47	l	703	PEE	C22-C23-C24-C25
53	i	401	CDL	C35-C36-C37-C38
53	l	702	CDL	C74-C75-C76-C77
53	l	701	CDL	C71-CB7-OB8-CB6
48	r	503	PLX	C31-C32-C33-C34
48	C	302	PLX	C13-C14-C15-C16
48	r	503	PLX	C9-C10-C11-C12
48	j	202	PLX	C9-C10-C11-C12
47	j	201	PEE	C1-C2-C3-O3
47	r	501	PEE	C1-C2-C3-O3
48	r	503	PLX	C3-C4-C5-O8
53	g	202	CDL	CA3-CA4-CA6-OA8
53	g	202	CDL	CB3-CB4-CB6-OB8
53	g	202	CDL	C74-C75-C76-C77
53	i	401	CDL	CB3-CB4-CB6-OB8
53	l	702	CDL	C31-C32-C33-C34
53	l	702	CDL	CB3-CB4-CB6-OB8
53	n	101	CDL	CA3-CA4-CA6-OA8
48	r	502	PLX	C15-C16-C17-C18
47	B	303	PEE	C23-C24-C25-C26
53	l	702	CDL	C14-C15-C16-C17
47	r	501	PEE	C20-C21-C22-C23
47	l	704	PEE	C15-C16-C17-C18
53	g	202	CDL	C79-C80-C81-C82
47	B	303	PEE	C21-C22-C23-C24
49	X	201	8Q1	C10-C11-C12-C13
53	n	101	CDL	C21-C22-C23-C24
53	a	201	CDL	C71-CB7-OB8-CB6
47	m	201	PEE	O3P-C1-C2-O2
48	C	302	PLX	O4-C3-C4-O6
48	j	202	PLX	C2-C1-N1-C1C
48	j	202	PLX	C2-C1-N1-C1B
53	g	202	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
53	i	401	CDL	C13-C14-C15-C16
53	l	702	CDL	C52-C53-C54-C55
47	m	201	PEE	C13-C14-C15-C16
49	X	201	8Q1	C13-C14-C15-C16
47	l	703	PEE	O2-C2-C3-O3
53	g	202	CDL	OA6-CA4-CA6-OA8
53	l	701	CDL	OB9-CB7-OB8-CB6
49	X	201	8Q1	C31-C29-C32-O33
53	g	202	CDL	C32-C33-C34-C35
47	l	704	PEE	C13-C14-C15-C16
53	g	202	CDL	C55-C56-C57-C58
47	l	704	PEE	C37-C38-C39-C40
48	r	502	PLX	C13-C14-C15-C16
53	l	702	CDL	C17-C18-C19-C20
48	g	201	PLX	C27-C28-C29-C30
48	r	503	PLX	C16-C17-C18-C19
48	r	503	PLX	C36-C37-C38-C39
49	X	201	8Q1	C29-C32-C34-O35
47	j	201	PEE	C13-C14-C15-C16
48	j	202	PLX	C33-C34-C35-C36
53	l	701	CDL	C72-C73-C74-C75
49	G	201	8Q1	N41-C42-C43-S44
48	g	201	PLX	C13-C14-C15-C16
53	g	202	CDL	C54-C55-C56-C57
53	g	202	CDL	C63-C64-C65-C66
53	l	701	CDL	C37-C38-C39-C40
48	r	502	PLX	C16-C17-C18-C19
53	g	202	CDL	C20-C21-C22-C23
47	l	704	PEE	C1-C2-C3-O3
47	m	201	PEE	C1-C2-C3-O3
48	r	502	PLX	C3-C4-C5-O8
53	l	702	CDL	CA3-CA4-CA6-OA8
48	C	302	PLX	C10-C11-C12-C13
48	r	502	PLX	C31-C32-C33-C34
53	l	701	CDL	C36-C37-C38-C39
53	l	702	CDL	C82-C83-C84-C85
48	r	503	PLX	O7-C6-C7-C8
48	r	503	PLX	C27-C28-C29-C30
48	a	202	PLX	O4-C3-C4-O6
48	r	502	PLX	O4-C3-C4-O6
47	j	201	PEE	C10-C11-C12-C13
53	l	702	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
53	l	702	CDL	C16-C17-C18-C19
48	a	202	PLX	C33-C34-C35-C36
48	r	503	PLX	C11-C12-C13-C14
47	m	201	PEE	O2-C2-C3-O3
47	r	501	PEE	O2-C2-C3-O3
48	r	502	PLX	O6-C4-C5-O8
53	g	202	CDL	C42-C43-C44-C45
53	n	101	CDL	CB2-C1-CA2-OA2
48	r	503	PLX	C19-C20-C21-C22
47	l	703	PEE	C33-C34-C35-C36
47	l	704	PEE	C22-C23-C24-C25
53	g	202	CDL	CB4-CB3-OB5-PB2
47	B	303	PEE	C15-C16-C17-C18
48	g	201	PLX	C14-C15-C16-C17
48	g	201	PLX	C29-C30-C31-C32
48	j	202	PLX	C14-C15-C16-C17
53	i	401	CDL	C71-C72-C73-C74
49	X	201	8Q1	O4-C1-S44-C43
48	g	201	PLX	C28-C29-C30-C31
53	g	202	CDL	C57-C58-C59-C60
53	l	702	CDL	C64-C65-C66-C67
47	i	402	PEE	C24-C25-C26-C27
53	l	702	CDL	C62-C63-C64-C65
49	X	201	8Q1	O4-C1-C6-C7
49	X	201	8Q1	S44-C1-C6-C7
47	m	201	PEE	C22-C23-C24-C25
48	C	302	PLX	O4-C3-C4-C5
48	j	202	PLX	O4-C3-C4-C5
47	B	303	PEE	C38-C39-C40-C41
47	B	303	PEE	C31-C30-O3-C3
53	g	202	CDL	C13-C14-C15-C16
49	X	201	8Q1	O33-C32-C34-N36
49	X	201	8Q1	C28-O27-P24-O1
49	X	201	8Q1	C6-C1-S44-C43
47	B	303	PEE	C33-C34-C35-C36
48	g	201	PLX	C3-C4-C5-O8
53	a	201	CDL	OB9-CB7-OB8-CB6
47	B	303	PEE	O3P-C1-C2-O2
53	l	702	CDL	OA5-CA3-CA4-OA6
48	g	201	PLX	C36-C37-C38-C39
47	l	704	PEE	O2-C2-C3-O3
48	g	201	PLX	O6-C4-C5-O8

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Mol	Chain	Res	Type	Atoms
48	r	503	PLX	O6-C4-C5-O8
53	n	101	CDL	OA6-CA4-CA6-OA8
47	r	501	PEE	C24-C25-C26-C27
53	l	702	CDL	C53-C54-C55-C56
53	g	202	CDL	C44-C45-C46-C47
50	J	401	NDP	C5B-O5B-PA-O3
47	i	402	PEE	C39-C40-C41-C42
53	l	702	CDL	C44-C45-C46-C47
47	B	303	PEE	O5-C30-O3-C3
53	g	202	CDL	C76-C77-C78-C79
47	r	501	PEE	C22-C23-C24-C25
48	a	202	PLX	C6-C7-C8-C9
47	i	402	PEE	C1-O3P-P-O4P
53	a	201	CDL	CA3-OA5-PA1-OA2
53	a	201	CDL	CB3-OB5-PB2-OB2
53	i	401	CDL	CB3-OB5-PB2-OB2
53	l	701	CDL	CB3-OB5-PB2-OB2
53	l	702	CDL	CA2-OA2-PA1-OA5
47	l	704	PEE	C21-C22-C23-C24
47	U	101	PEE	C1-O3P-P-O2P
47	i	402	PEE	C1-O3P-P-O1P
47	l	704	PEE	C1-O3P-P-O2P
47	l	704	PEE	C1-O3P-P-O1P
47	m	201	PEE	C4-O4P-P-O2P
47	m	201	PEE	C4-O4P-P-O1P
47	r	501	PEE	C1-O3P-P-O2P
47	r	501	PEE	C1-O3P-P-O1P
48	j	202	PLX	C3-O4-P1-O3
53	N	201	CDL	CB3-OB5-PB2-OB4
53	a	201	CDL	CA2-OA2-PA1-OA4
53	a	201	CDL	CB2-OB2-PB2-OB4
53	g	202	CDL	CB2-OB2-PB2-OB4
53	g	202	CDL	CB3-OB5-PB2-OB3
53	i	401	CDL	CA3-OA5-PA1-OA4
53	i	401	CDL	CB2-OB2-PB2-OB3
53	l	701	CDL	CB3-OB5-PB2-OB4
53	l	702	CDL	CB3-OB5-PB2-OB3
53	l	702	CDL	CB3-OB5-PB2-OB4
53	n	101	CDL	CB3-OB5-PB2-OB4
48	j	202	PLX	C34-C35-C36-C37
47	m	201	PEE	O3P-C1-C2-C3
48	g	201	PLX	O4-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
53	l	702	CDL	OA5-CA3-CA4-CA6
53	g	202	CDL	C64-C65-C66-C67
49	G	201	8Q1	C11-C10-C9-C8
48	r	502	PLX	C12-C13-C14-C15
53	a	201	CDL	C54-C55-C56-C57
53	n	101	CDL	CB7-C71-C72-C73
48	j	202	PLX	O4-C3-C4-O6
53	l	701	CDL	CA7-C31-C32-C33
53	n	101	CDL	OB5-CB3-CB4-OB6
53	i	401	CDL	C14-C15-C16-C17
48	r	503	PLX	C15-C16-C17-C18
48	r	503	PLX	C7-C8-C9-C10
53	n	101	CDL	O1-C1-CA2-OA2
47	B	303	PEE	C12-C13-C14-C15
53	l	702	CDL	C56-C57-C58-C59
47	j	201	PEE	O2-C2-C3-O3
53	n	101	CDL	C73-C74-C75-C76
53	a	201	CDL	C17-C18-C19-C20
53	l	701	CDL	C40-C41-C42-C43
48	C	302	PLX	C31-C32-C33-C34
48	C	302	PLX	O6-C6-C7-C8
48	a	202	PLX	O8-C24-C25-C26
48	r	503	PLX	O8-C24-C25-C26
47	U	101	PEE	C38-C39-C40-C41
47	l	704	PEE	C16-C17-C18-C19
48	C	302	PLX	O7-C6-C7-C8
48	j	202	PLX	C11-C12-C13-C14
48	r	502	PLX	C11-C12-C13-C14
48	r	502	PLX	C18-C19-C20-C21
47	m	201	PEE	C31-C32-C33-C34
53	a	201	CDL	CA6-CA4-OA6-CA5
48	a	202	PLX	O4-C3-C4-C5
48	r	502	PLX	O4-C3-C4-C5
46	A	502	FMN	C5'-O5'-P-O1P
47	l	704	PEE	C2-C1-O3P-P
49	G	201	8Q1	C28-O27-P24-O3
49	X	201	8Q1	C28-O27-P24-O3
48	g	201	PLX	O4-C3-C4-O6
47	r	501	PEE	C31-C32-C33-C34
53	g	202	CDL	C34-C35-C36-C37
50	J	401	NDP	O4D-C1D-N1N-C6N
47	U	101	PEE	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
48	j	202	PLX	C31-C32-C33-C34
47	B	303	PEE	C34-C35-C36-C37
47	i	402	PEE	C31-C32-C33-C34
48	a	202	PLX	C2-O1-P1-O4
48	g	201	PLX	C3-O4-P1-O1
53	n	101	CDL	C55-C56-C57-C58
47	l	703	PEE	C1-C2-C3-O3
48	C	302	PLX	C11-C10-C9-C8
53	l	702	CDL	C60-C61-C62-C63
53	N	201	CDL	CB7-C71-C72-C73
53	l	702	CDL	C76-C77-C78-C79
53	l	702	CDL	C31-CA7-OA8-CA6
48	a	202	PLX	C26-C27-C28-C29
47	i	402	PEE	C38-C39-C40-C41
47	l	704	PEE	C36-C37-C38-C39
47	m	201	PEE	C16-C17-C18-C19
55	s	401	UQ	C17-C18-C19-C20
53	l	701	CDL	C76-C77-C78-C79
53	l	702	CDL	OA9-CA7-OA8-CA6
47	j	201	PEE	C31-C30-O3-C3
53	l	702	CDL	C32-C33-C34-C35
53	n	101	CDL	C22-C23-C24-C25
47	j	201	PEE	O5-C30-O3-C3
53	a	201	CDL	OA5-CA3-CA4-OA6
53	n	101	CDL	OA5-CA3-CA4-OA6
47	j	201	PEE	C16-C17-C18-C19
47	l	704	PEE	C38-C39-C40-C41
48	C	302	PLX	C11-C12-C13-C14
53	l	701	CDL	C17-C18-C19-C20
48	j	202	PLX	C18-C19-C20-C21
53	g	202	CDL	C31-CA7-OA8-CA6
47	j	201	PEE	C43-C44-C45-C46
49	X	201	8Q1	C29-C32-C34-N36
48	g	201	PLX	C6-C7-C8-C9
53	i	401	CDL	CA6-CA4-OA6-CA5
53	l	701	CDL	C54-C55-C56-C57
53	l	702	CDL	C41-C42-C43-C44
47	l	703	PEE	C32-C33-C34-C35
48	j	202	PLX	C3-C4-O6-C6
53	a	201	CDL	CA7-C31-C32-C33
47	m	201	PEE	O3-C30-C31-C32
47	l	703	PEE	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
48	a	202	PLX	C13-C14-C15-C16
53	l	701	CDL	C44-C45-C46-C47
47	B	303	PEE	O3P-C1-C2-C3
48	r	503	PLX	C26-C27-C28-C29
53	l	701	CDL	C34-C35-C36-C37
53	g	202	CDL	CA5-C11-C12-C13
47	U	101	PEE	O2-C2-C3-O3
47	i	402	PEE	C32-C33-C34-C35
53	l	701	CDL	C23-C24-C25-C26
53	g	202	CDL	OA9-CA7-OA8-CA6
53	N	201	CDL	CB2-C1-CA2-OA2
55	s	401	UQ	C14-C16-C17-C18
53	g	202	CDL	C60-C61-C62-C63
48	C	302	PLX	C12-C13-C14-C15
50	J	401	NDP	PN-O3-PA-O1A
50	J	401	NDP	PN-O3-PA-O2A
53	N	201	CDL	OA9-CA7-OA8-CA6
47	i	402	PEE	C17-C18-C19-C20
47	B	303	PEE	C18-C19-C20-C21
48	a	202	PLX	C9-C10-C11-C12
53	l	701	CDL	C42-C43-C44-C45
53	n	101	CDL	C71-C72-C73-C74
47	l	704	PEE	C12-C13-C14-C15
47	m	201	PEE	C24-C25-C26-C27
47	r	501	PEE	C38-C39-C40-C41
53	l	701	CDL	OA6-CA4-CA6-OA8
53	N	201	CDL	C31-CA7-OA8-CA6
47	j	201	PEE	C44-C45-C46-C47
47	U	101	PEE	C43-C44-C45-C46
47	U	101	PEE	O3-C30-C31-C32
47	B	303	PEE	C16-C17-C18-C19
47	l	703	PEE	C18-C19-C20-C21
53	l	701	CDL	C12-C11-CA5-OA6
53	n	101	CDL	C77-C78-C79-C80
47	j	201	PEE	C38-C39-C40-C41
47	i	402	PEE	C1-C2-C3-O3
48	j	202	PLX	C7-C6-O6-C4
56	w	401	ADP	C4'-C5'-O5'-PA
47	l	703	PEE	O3P-C1-C2-O2
53	i	401	CDL	OA5-CA3-CA4-OA6
47	l	703	PEE	C17-C18-C19-C20
47	j	201	PEE	O3-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
53	l	702	CDL	C12-C11-CA5-OA6
47	B	303	PEE	C24-C25-C26-C27
53	g	202	CDL	C80-C81-C82-C83
53	l	702	CDL	C71-C72-C73-C74
53	i	401	CDL	OA5-CA3-CA4-CA6
53	n	101	CDL	OB5-CB3-CB4-CB6
47	i	402	PEE	O2-C2-C3-O3
53	N	201	CDL	OB6-CB4-CB6-OB8
47	l	703	PEE	C36-C37-C38-C39
53	l	702	CDL	C32-C31-CA7-OA8
48	a	202	PLX	O7-C6-C7-C8
50	J	401	NDP	C2B-O2B-P2B-O2X
48	a	202	PLX	C10-C11-C12-C13
47	i	402	PEE	C2-C1-O3P-P
47	U	101	PEE	C16-C17-C18-C19
47	i	402	PEE	C36-C37-C38-C39
47	m	201	PEE	C18-C19-C20-C21
47	i	402	PEE	C18-C19-C20-C21
47	l	703	PEE	C16-C17-C18-C19
53	g	202	CDL	C83-C84-C85-C86
53	a	201	CDL	C71-C72-C73-C74
47	j	201	PEE	O5-C30-C31-C32
53	l	702	CDL	C12-C11-CA5-OA7
48	j	202	PLX	C11-C10-C9-C8
53	l	702	CDL	C32-C31-CA7-OA9
53	N	201	CDL	C31-C32-C33-C34
47	j	201	PEE	C4-O4P-P-O2P
47	l	703	PEE	C1-O3P-P-O2P
48	a	202	PLX	C2-O1-P1-O2
48	j	202	PLX	C3-O4-P1-O2
53	l	701	CDL	CB3-OB5-PB2-OB3
53	l	701	CDL	C12-C11-CA5-OA7
47	U	101	PEE	O5-C30-C31-C32
49	G	201	8Q1	C29-C32-C34-O35
47	l	703	PEE	C13-C14-C15-C16
47	l	704	PEE	C31-C32-C33-C34
53	l	702	CDL	C77-C78-C79-C80
47	l	704	PEE	C20-C21-C22-C23
53	n	101	CDL	C12-C11-CA5-OA6
47	r	501	PEE	C40-C41-C42-C43
53	g	202	CDL	C52-C51-CB5-OB6
53	l	702	CDL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
48	r	503	PLX	C24-C25-C26-C27
47	U	101	PEE	O2-C10-C11-C12

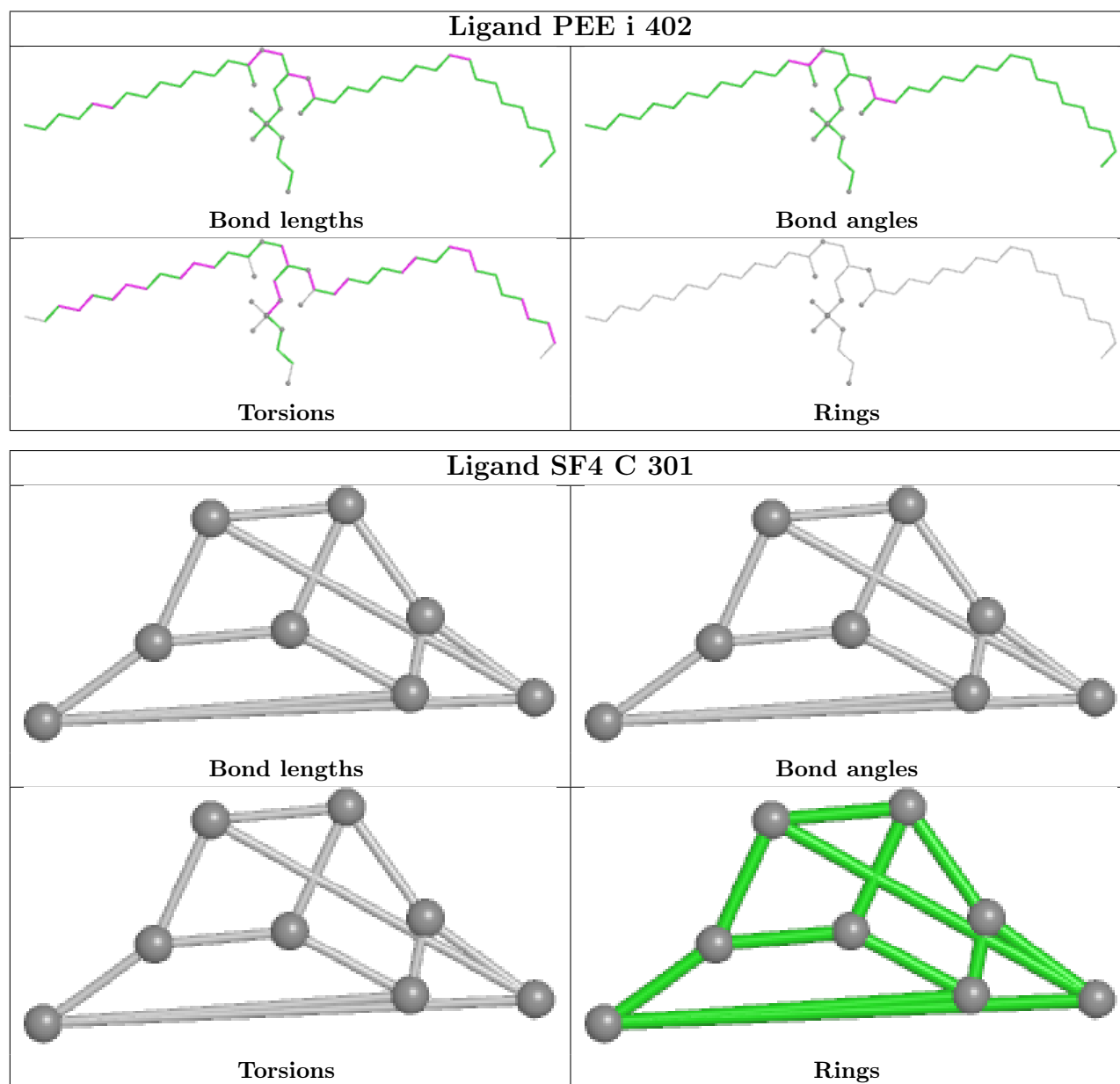
There are no ring outliers.

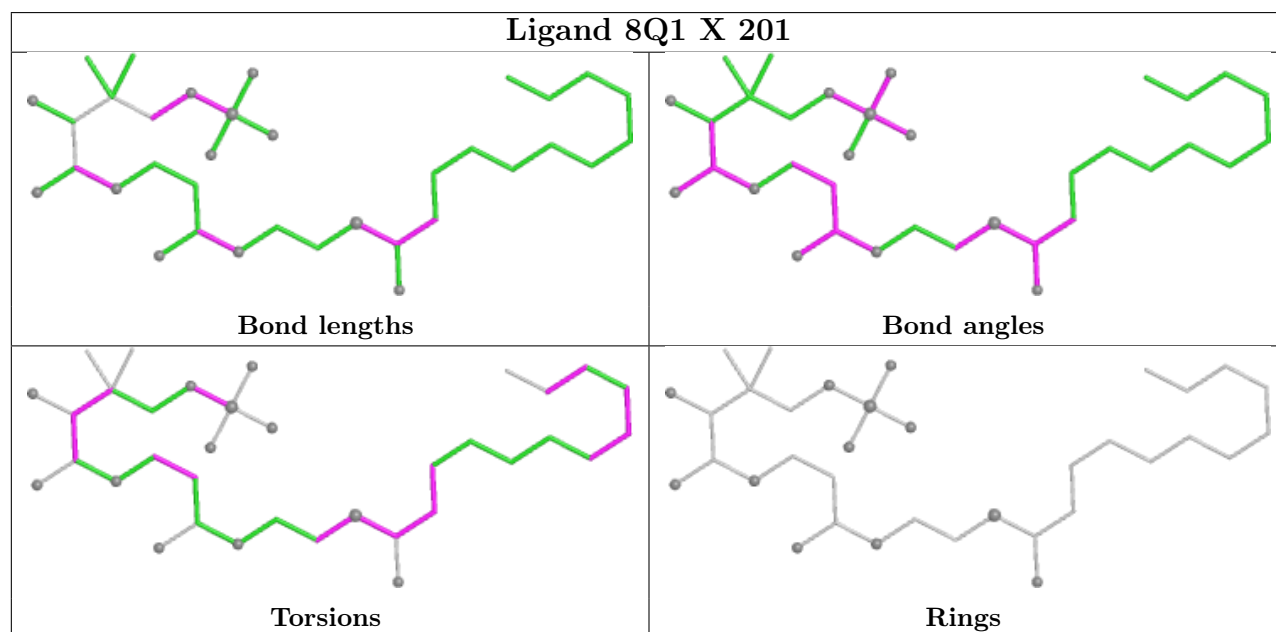
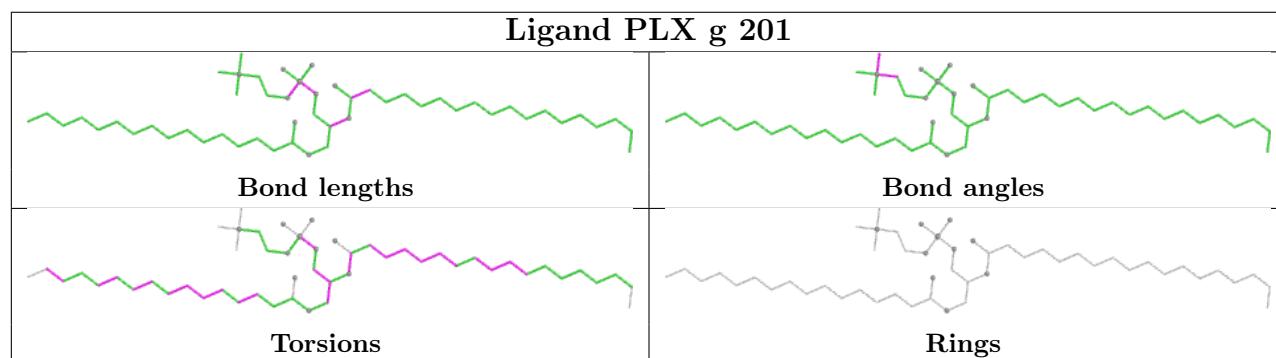
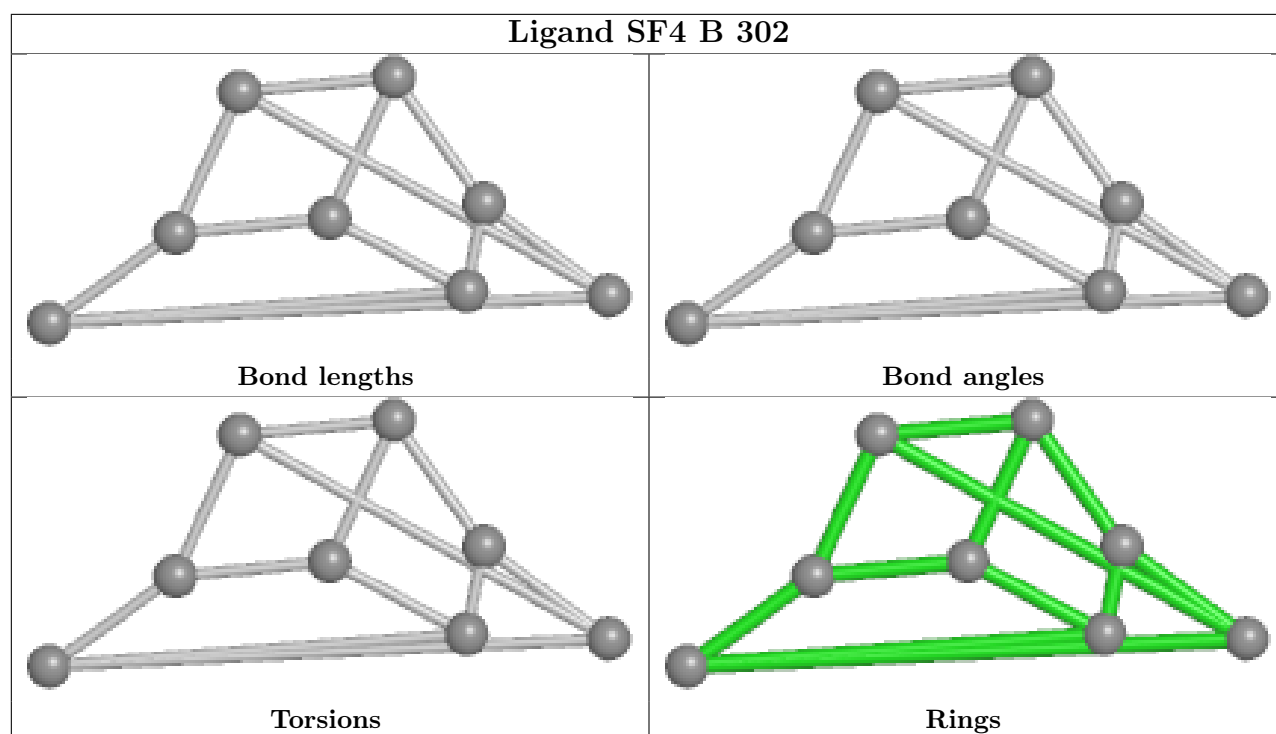
28 monomers are involved in 267 short contacts:

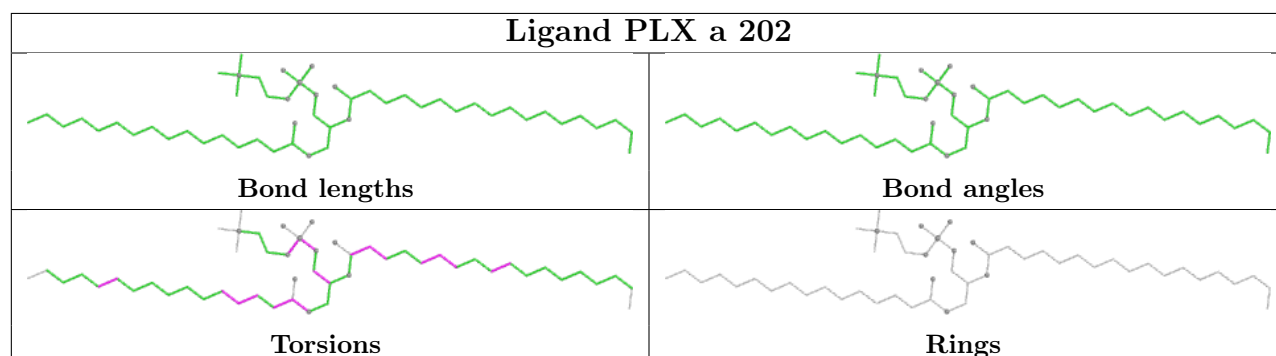
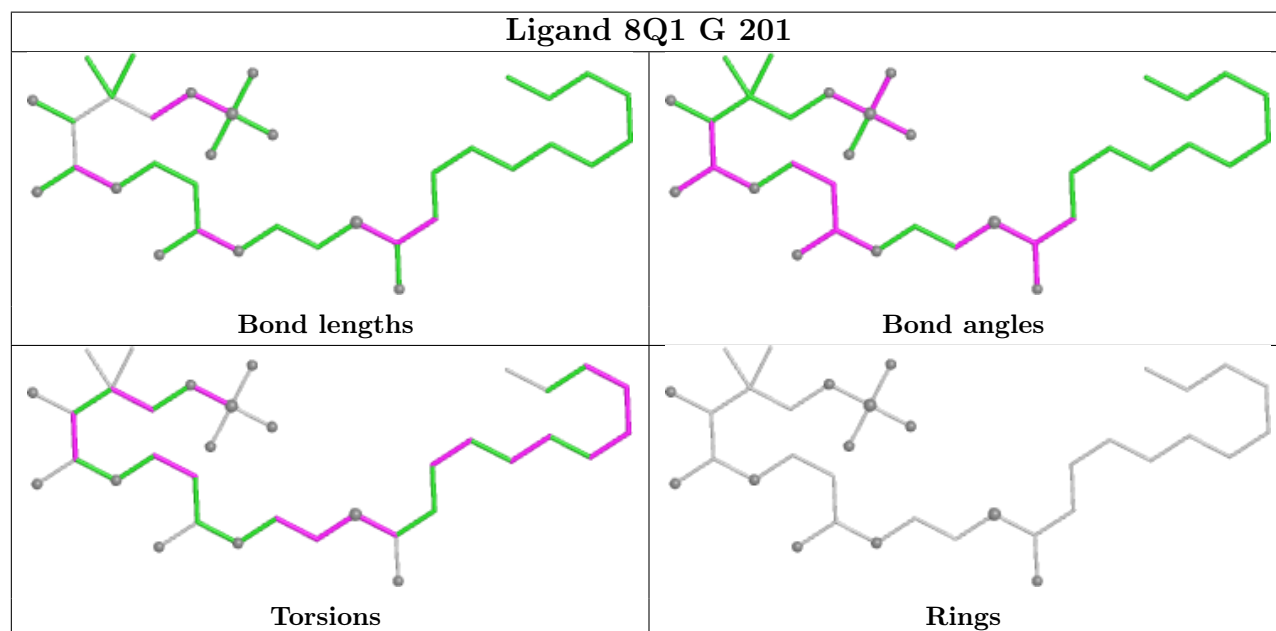
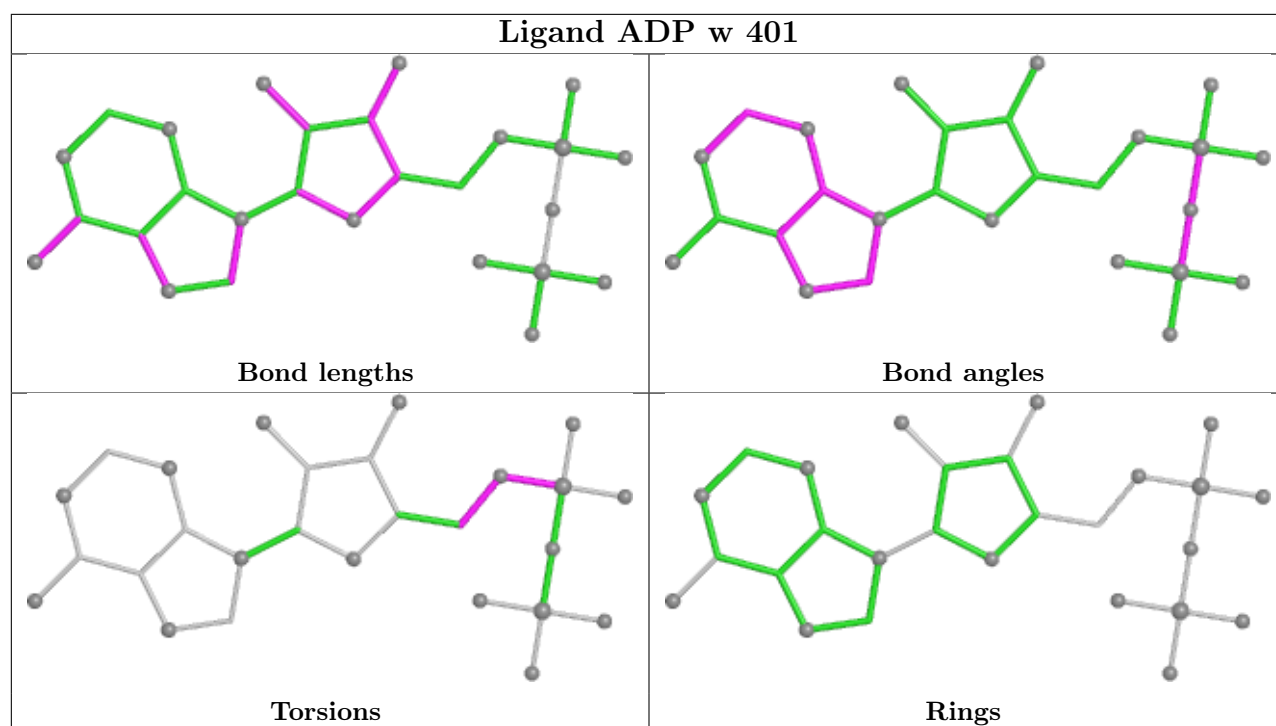
Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	i	402	PEE	18	0
45	C	301	SF4	1	0
48	g	201	PLX	5	0
49	X	201	8Q1	2	0
56	w	401	ADP	13	0
48	a	202	PLX	11	0
48	r	502	PLX	3	0
47	l	704	PEE	33	0
45	A	501	SF4	2	0
53	l	702	CDL	7	0
55	s	401	UQ	7	0
47	r	501	PEE	5	0
46	A	502	FMN	5	0
50	J	401	NDP	8	0
47	l	703	PEE	5	0
53	i	401	CDL	13	0
53	n	101	CDL	20	0
53	g	202	CDL	7	0
53	l	701	CDL	13	0
53	a	201	CDL	26	0
47	U	101	PEE	6	0
47	B	303	PEE	6	0
47	m	201	PEE	23	0
48	j	202	PLX	4	0
48	C	302	PLX	4	0
53	N	201	CDL	13	0
48	r	503	PLX	4	0
47	j	201	PEE	18	0

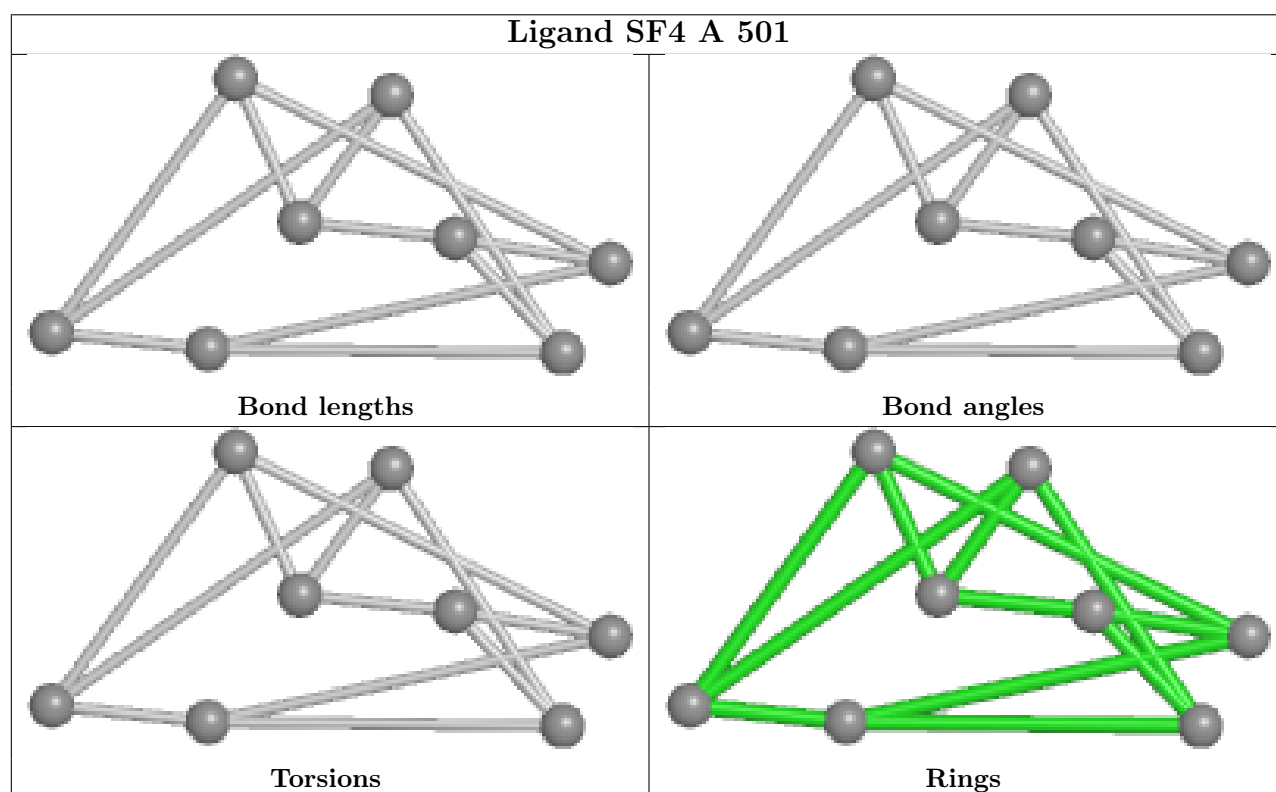
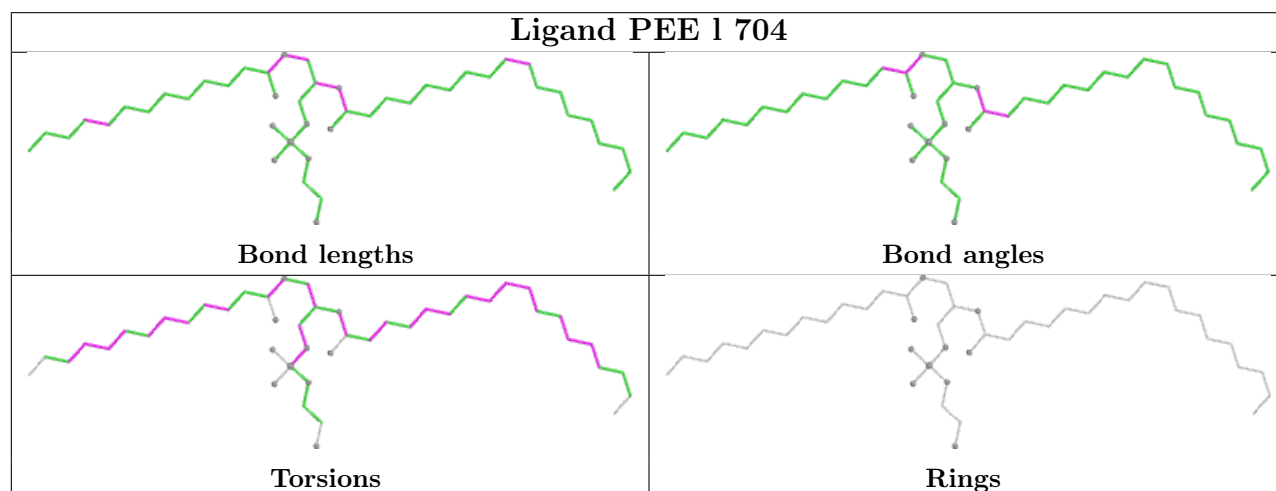
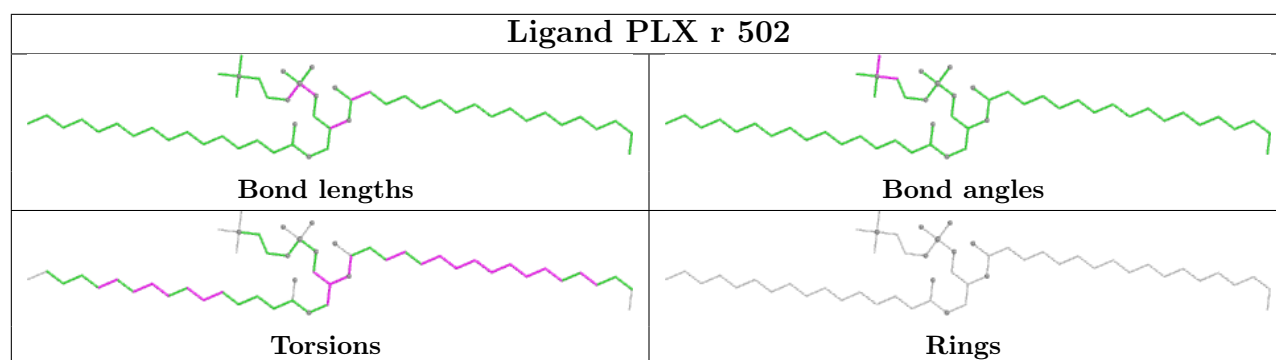
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

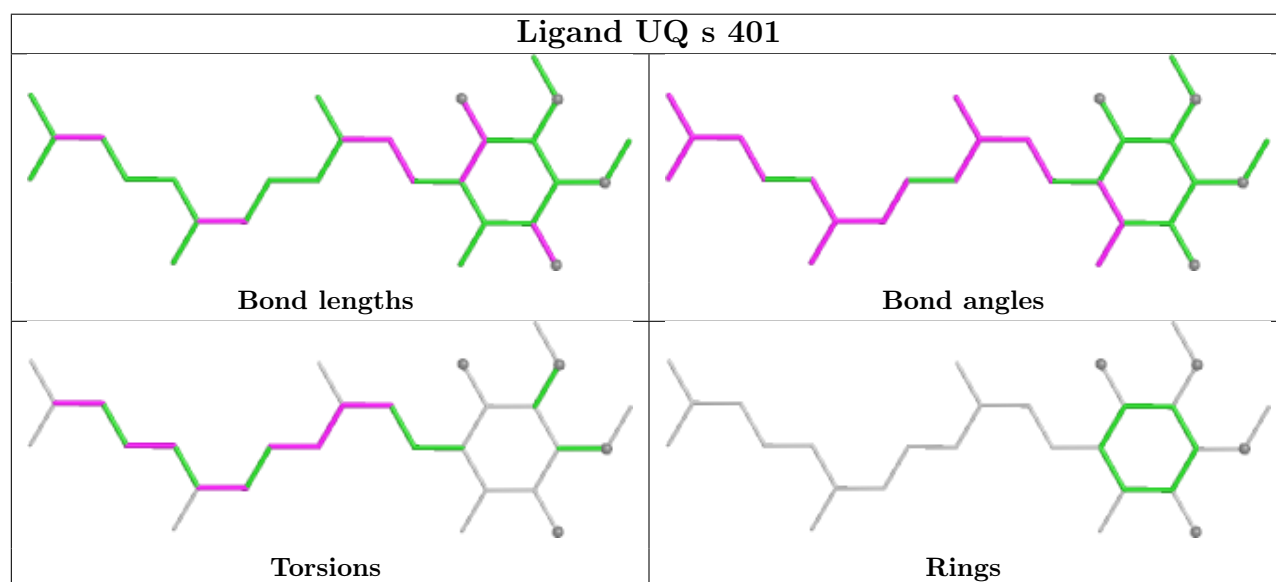
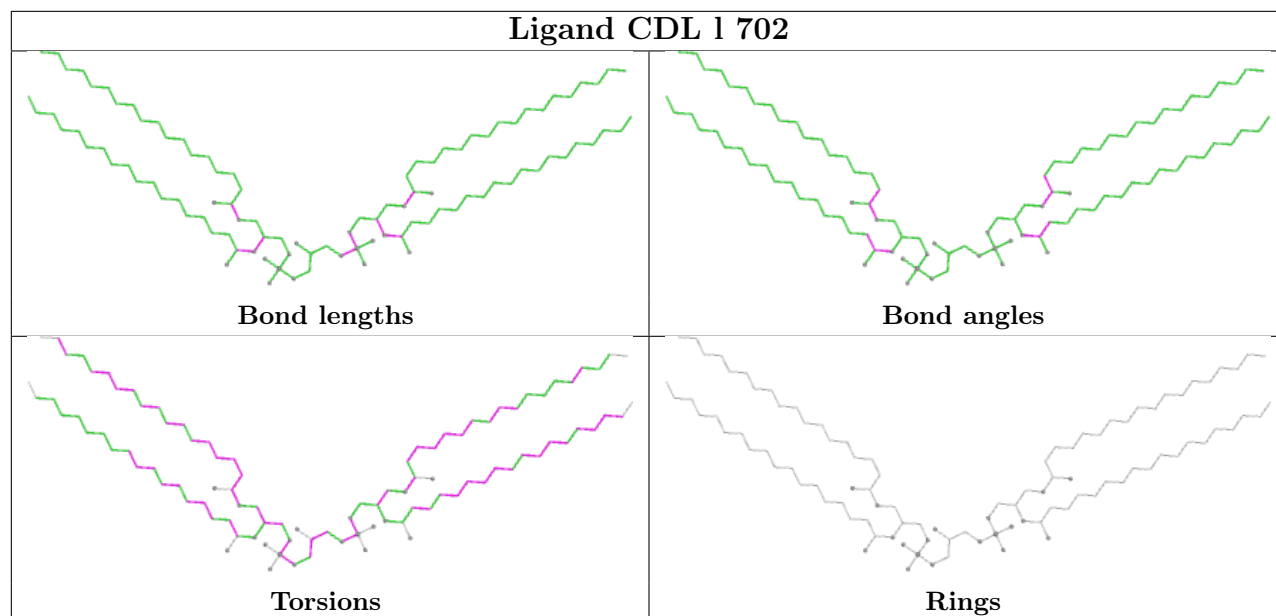
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

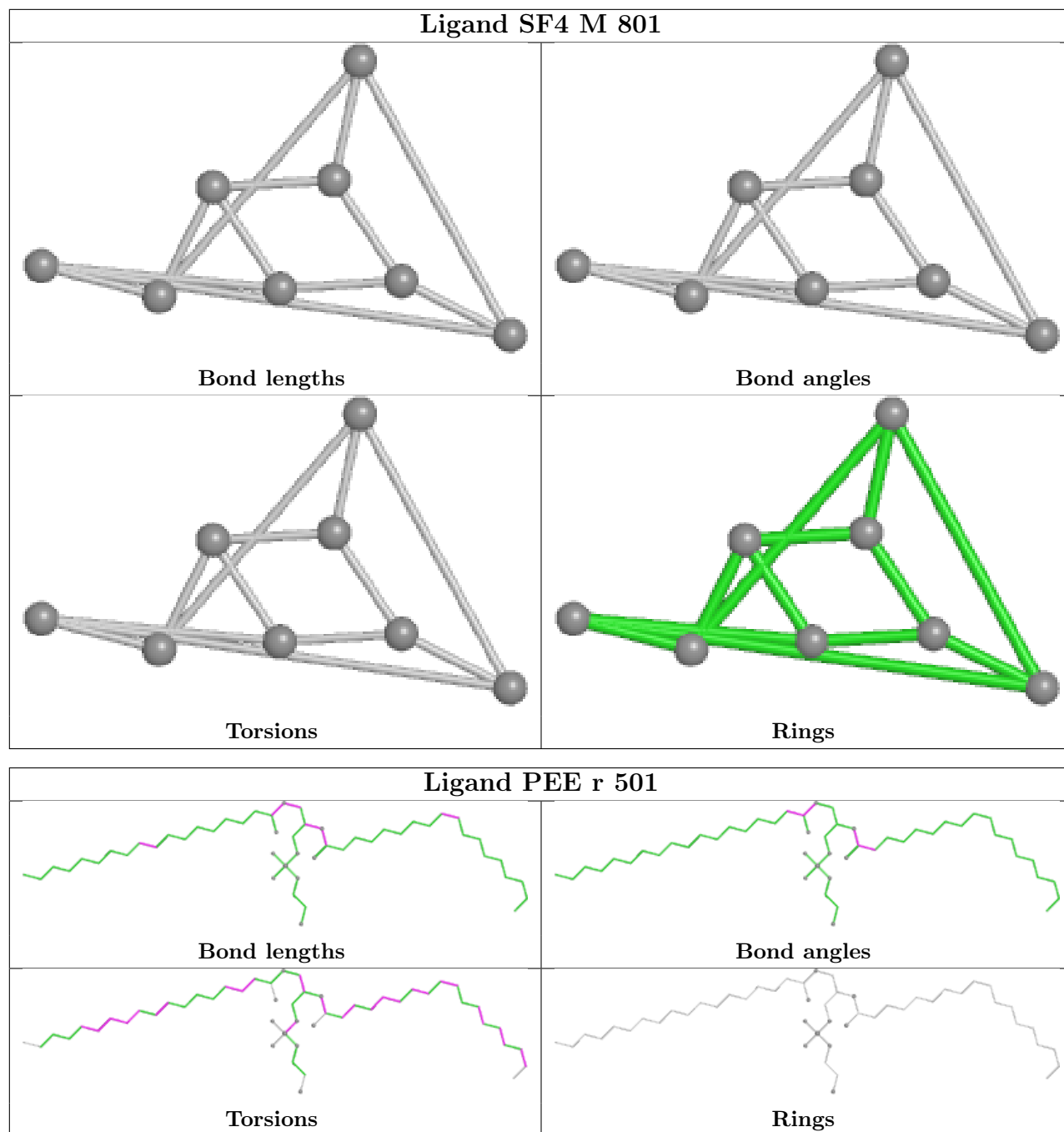


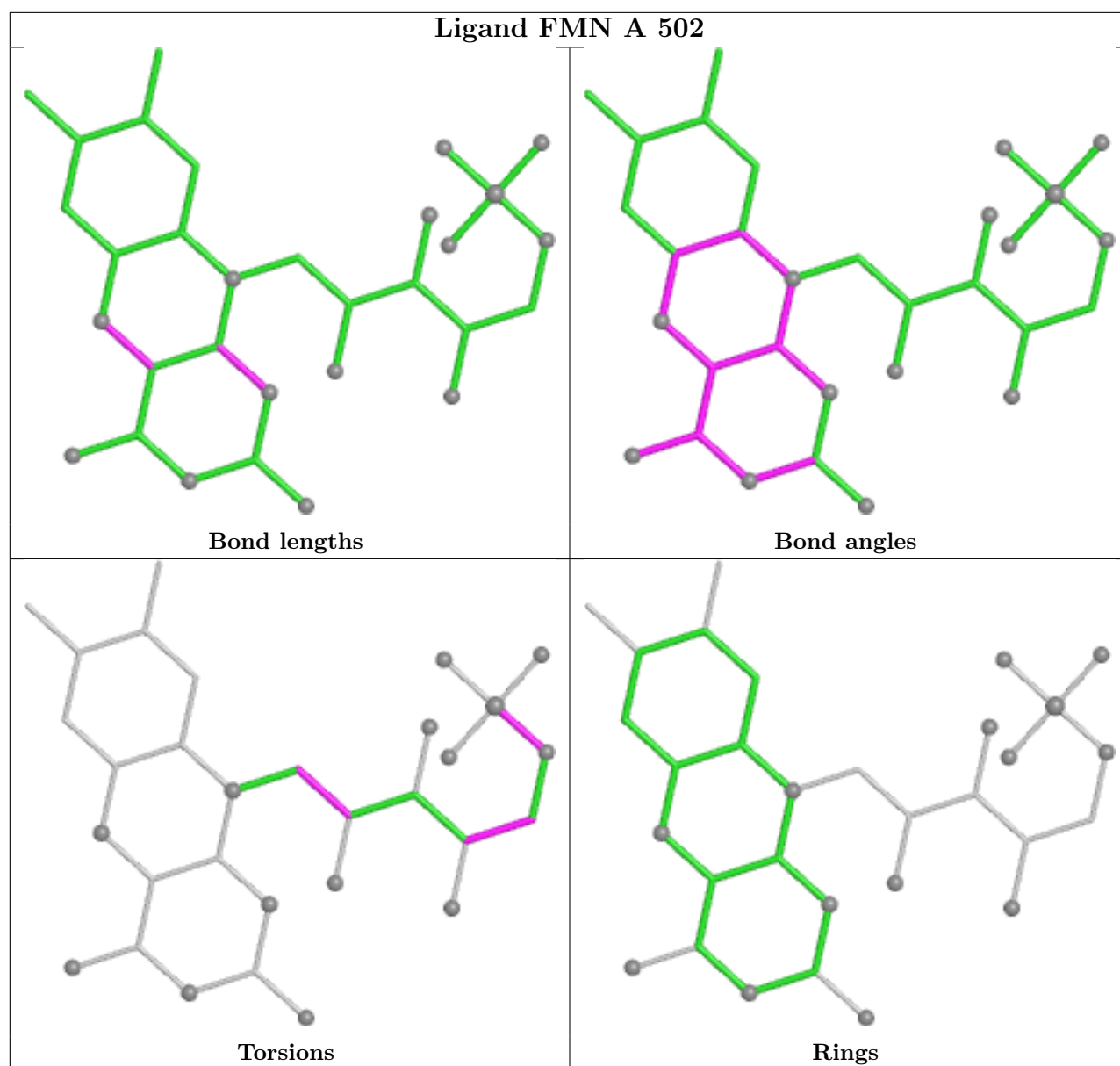


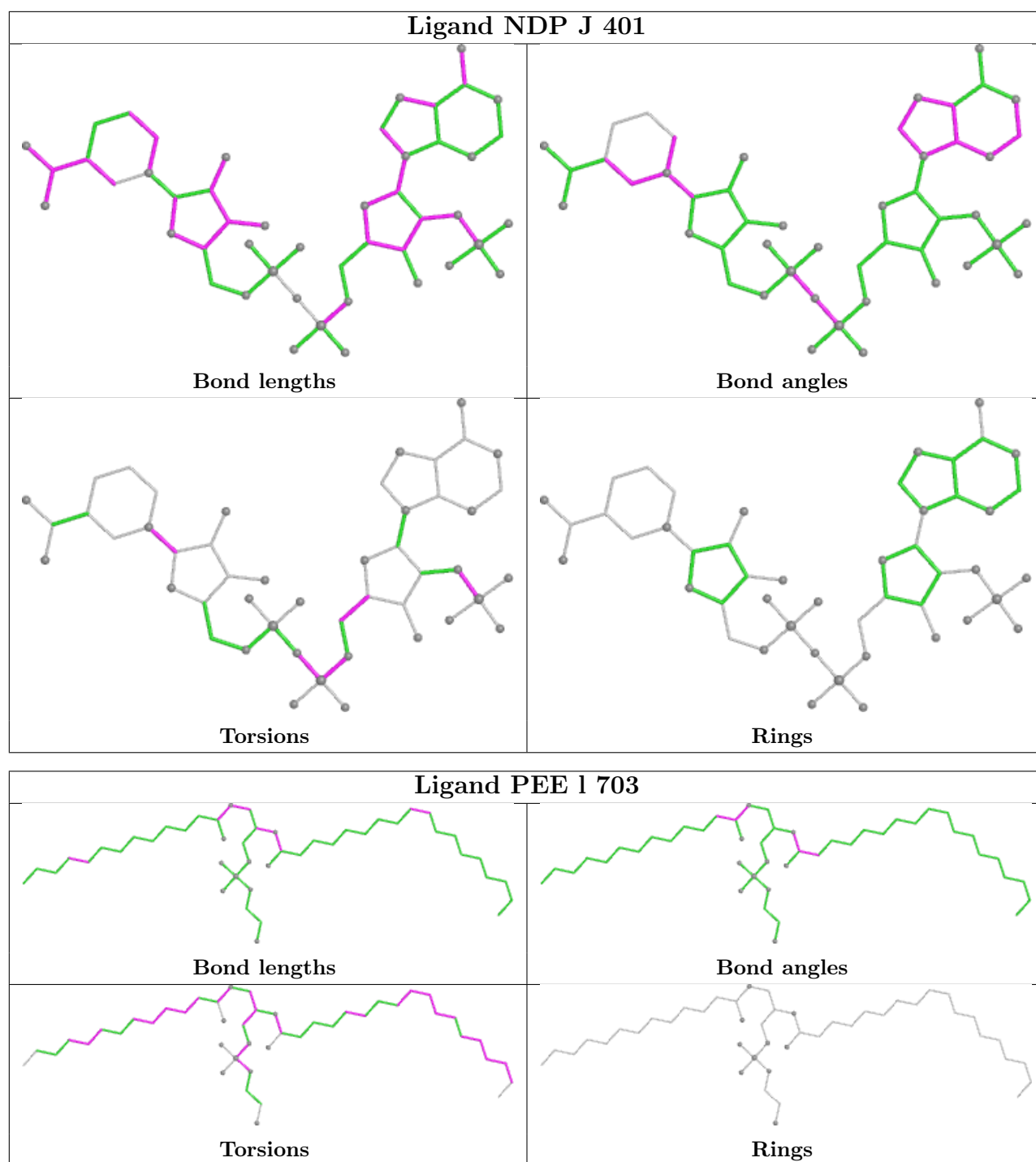


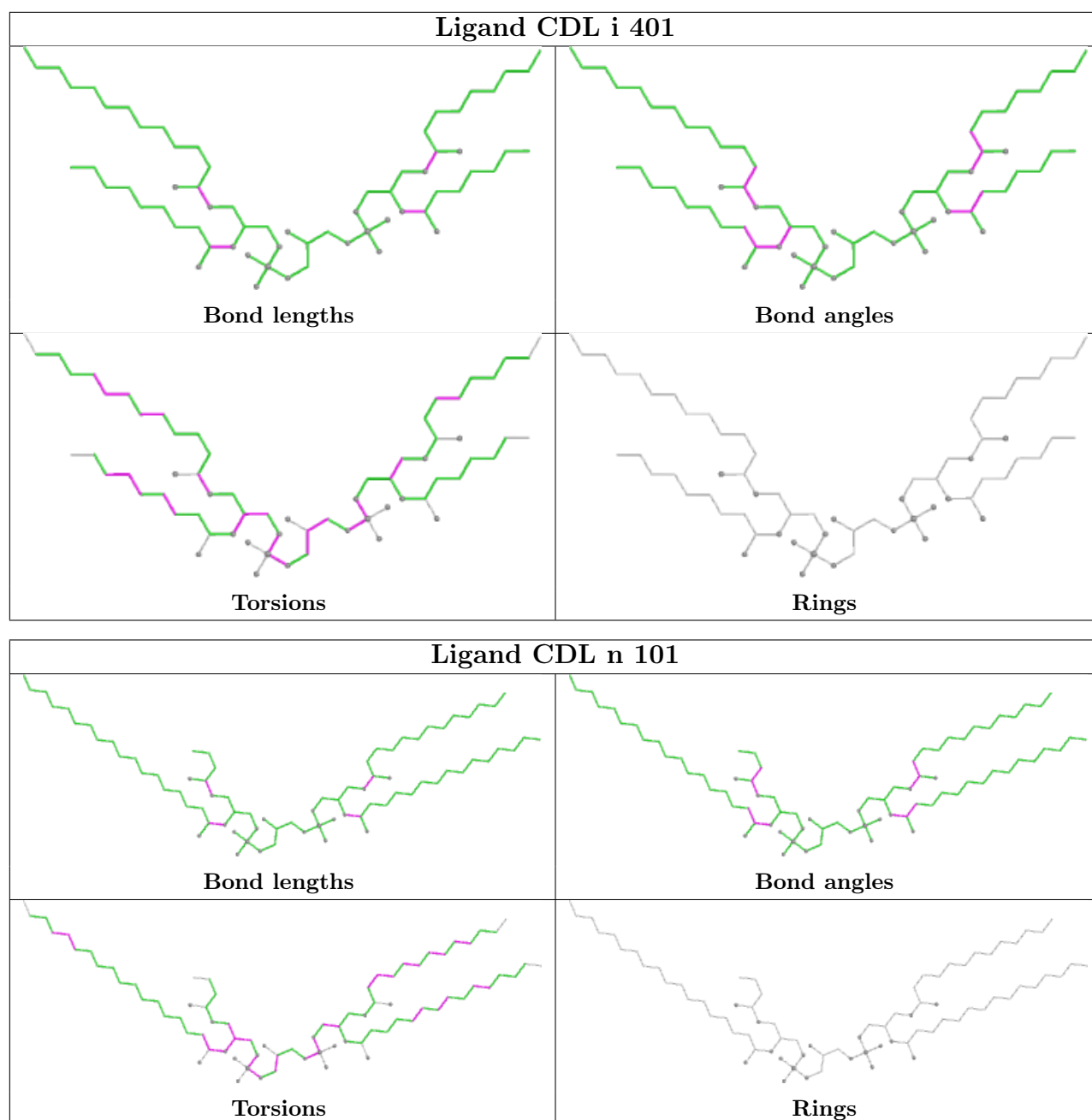


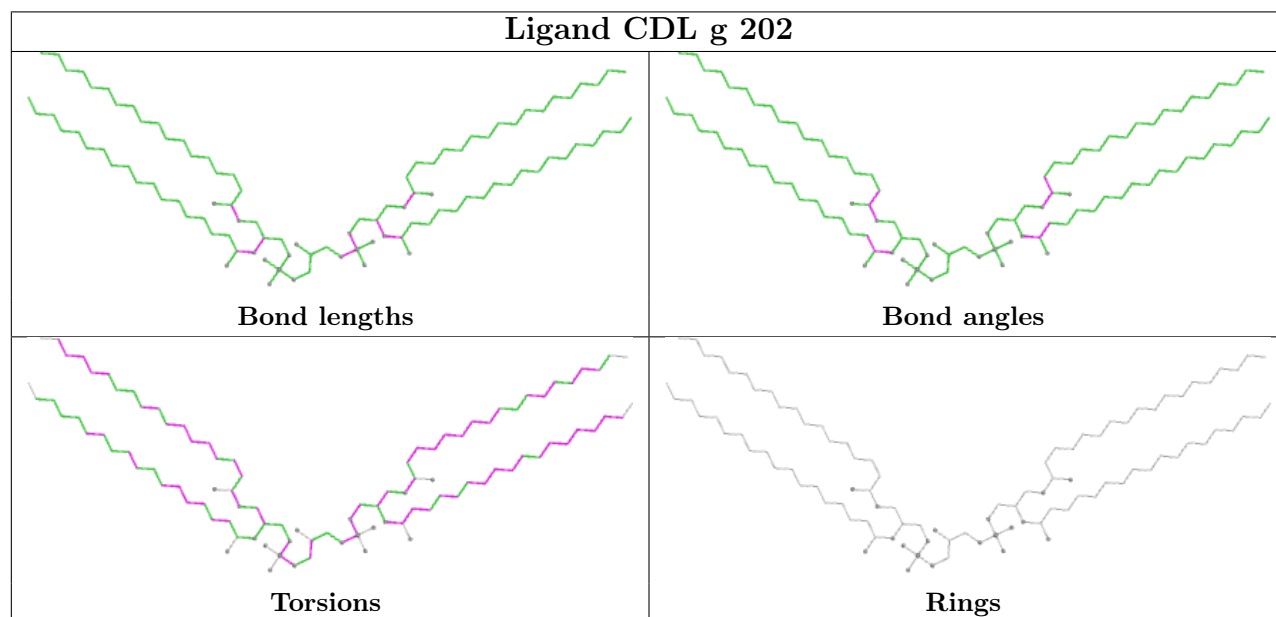
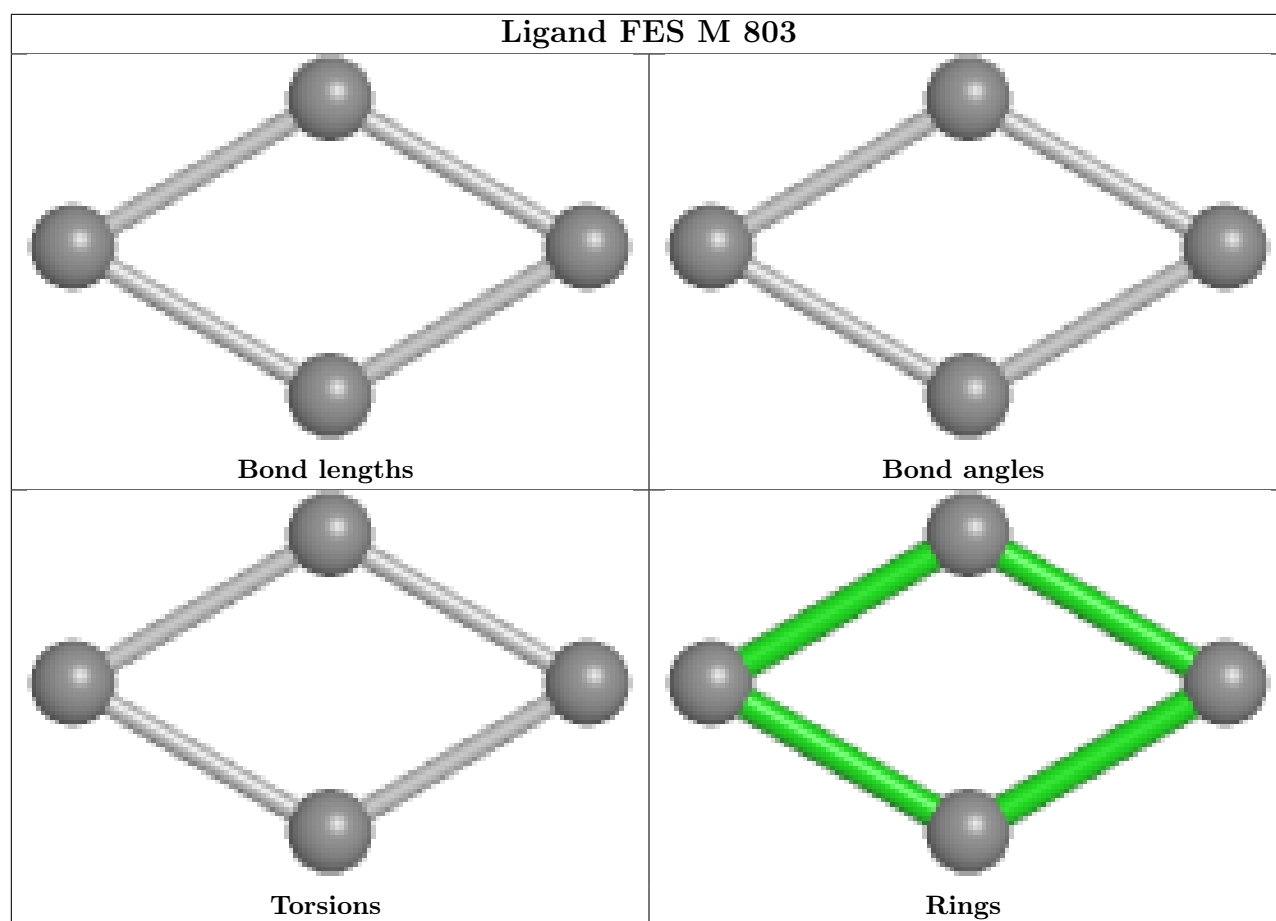


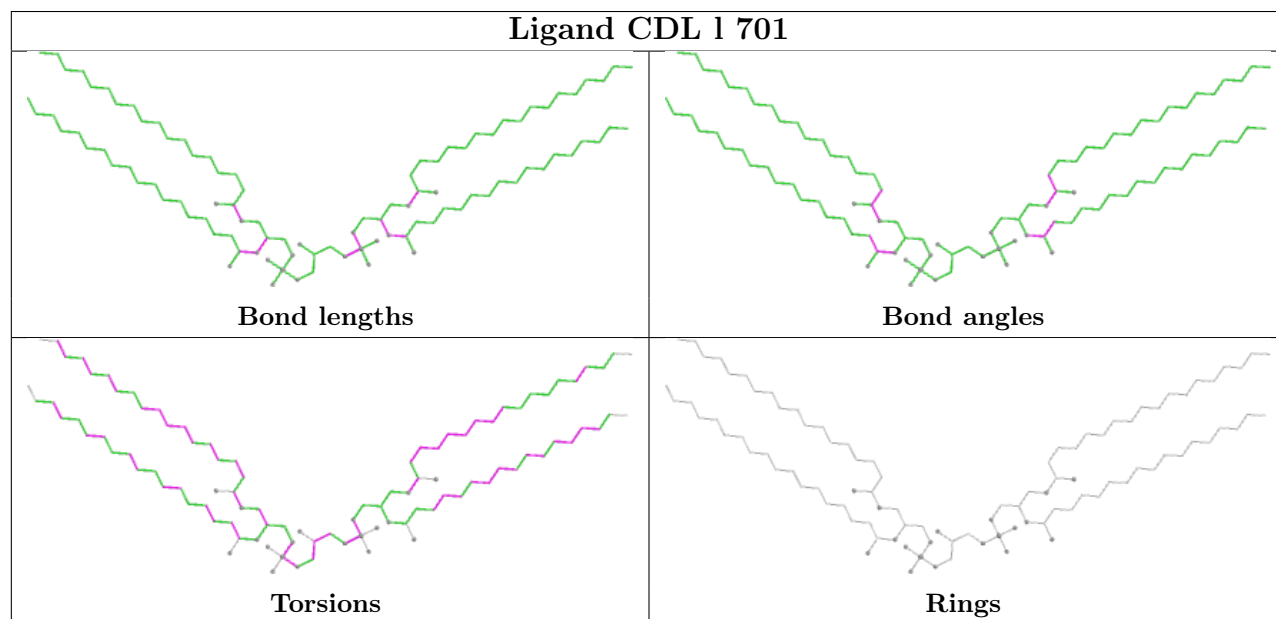
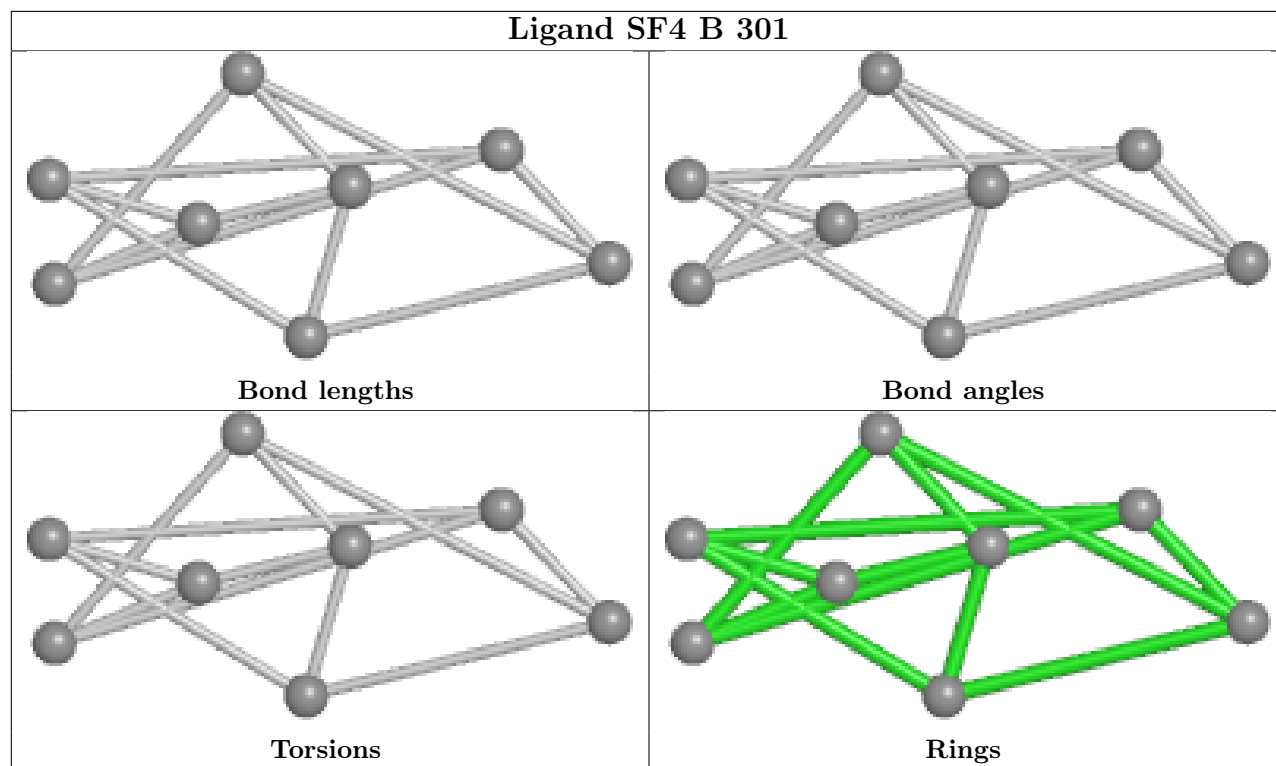


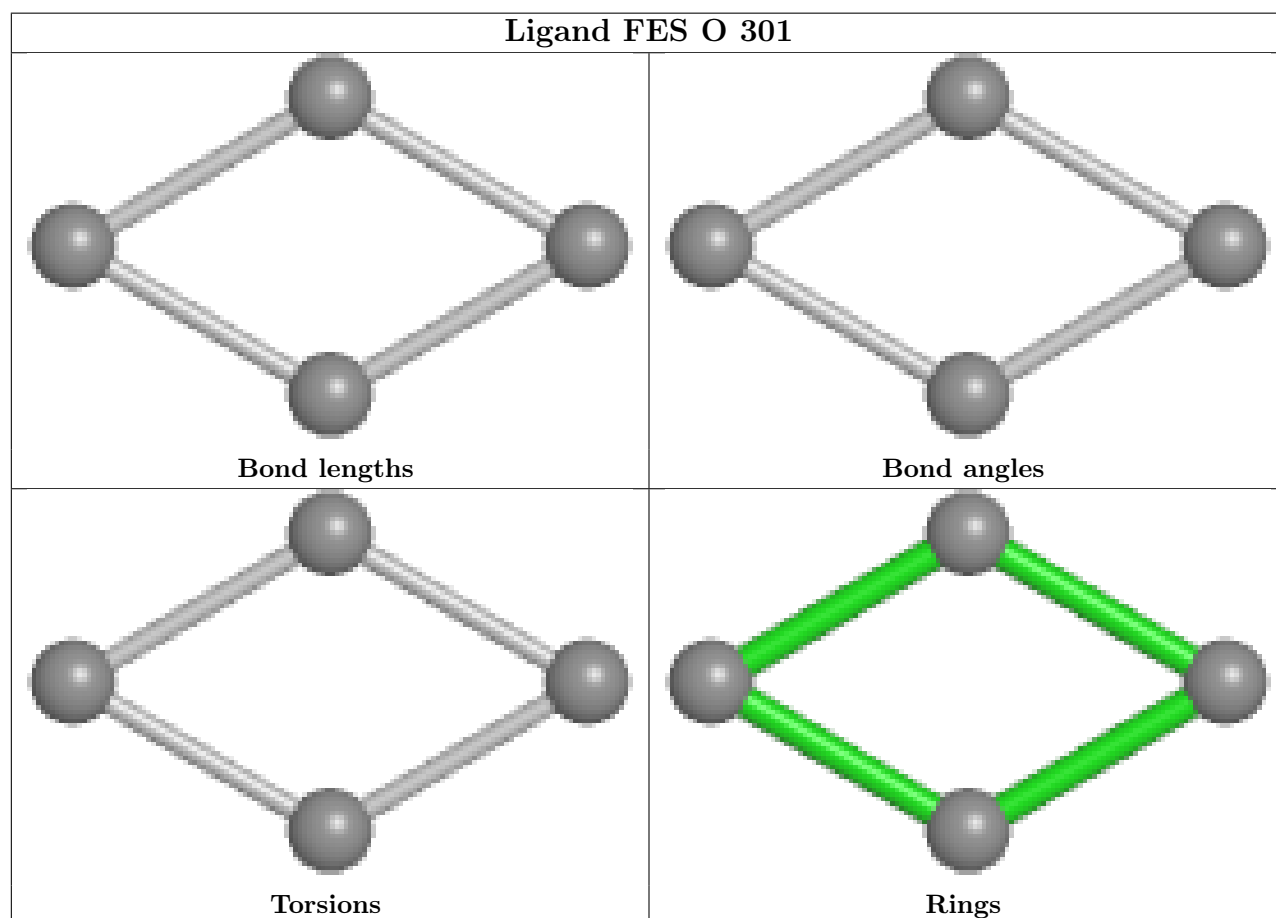
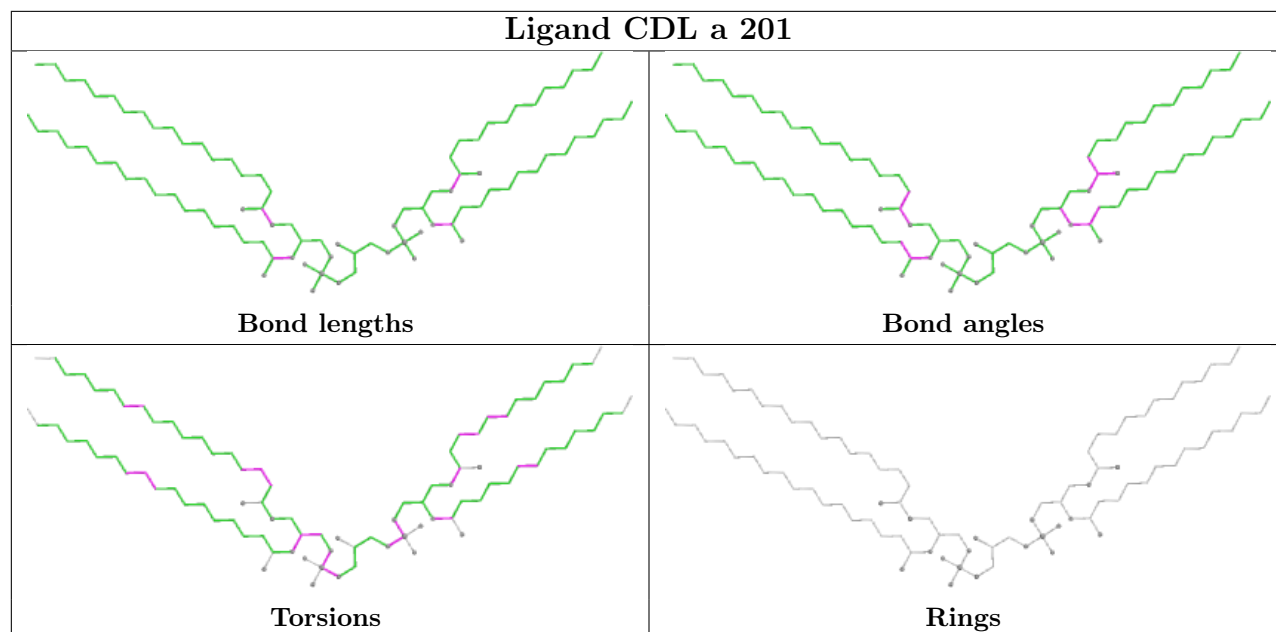


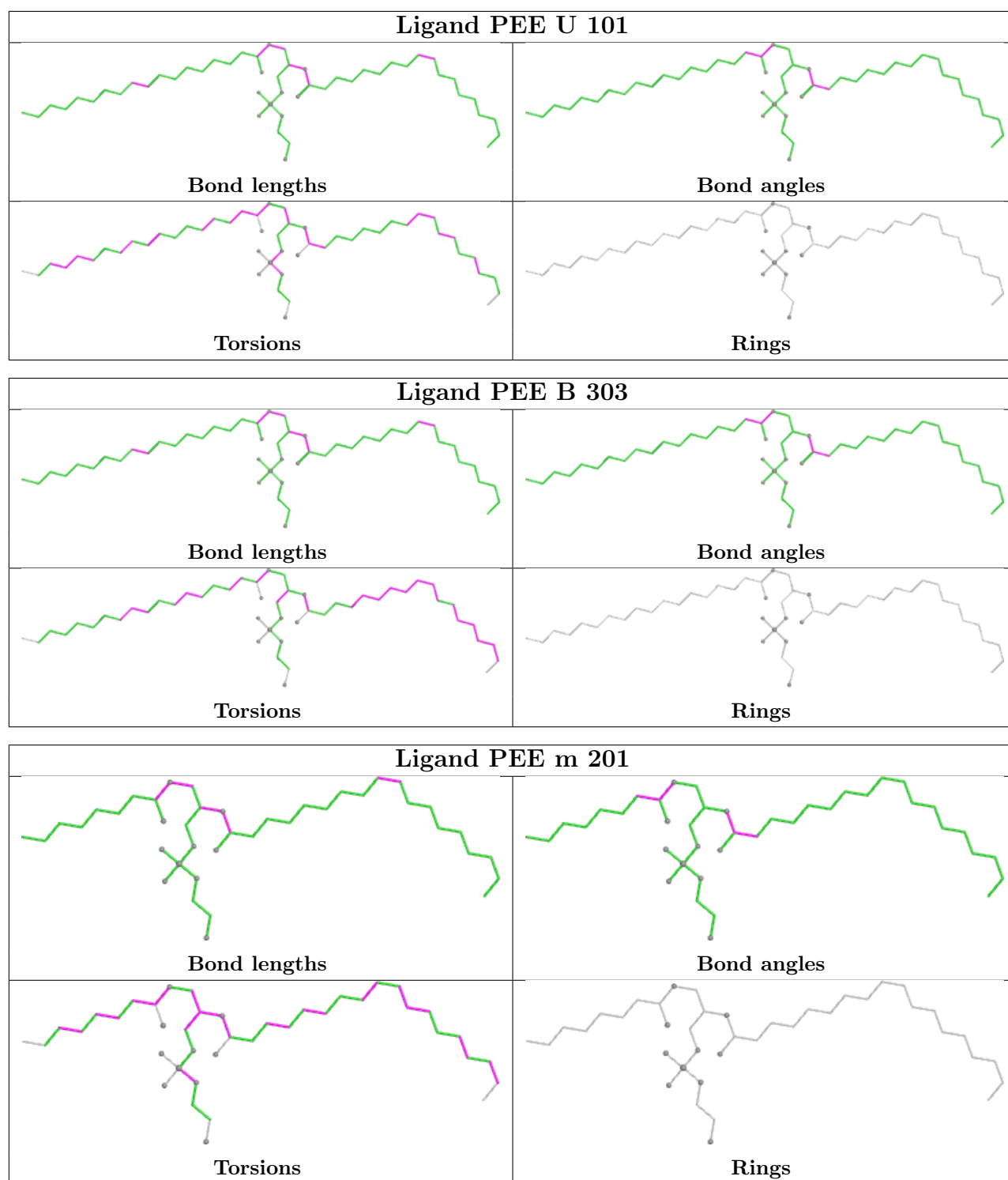


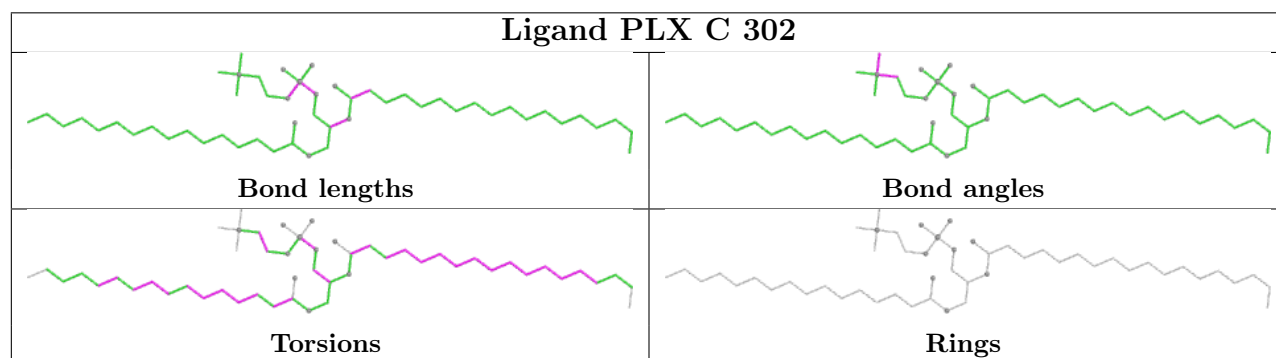
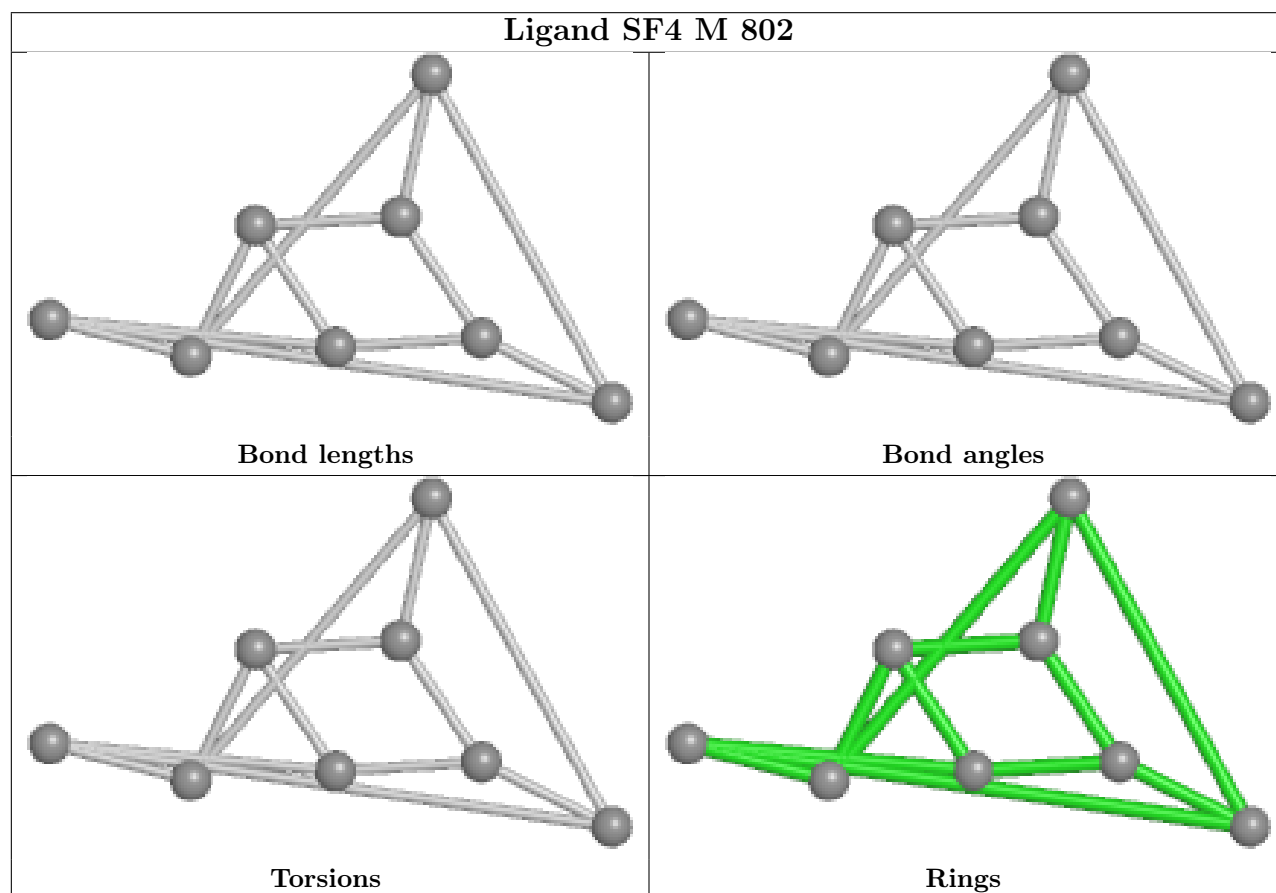
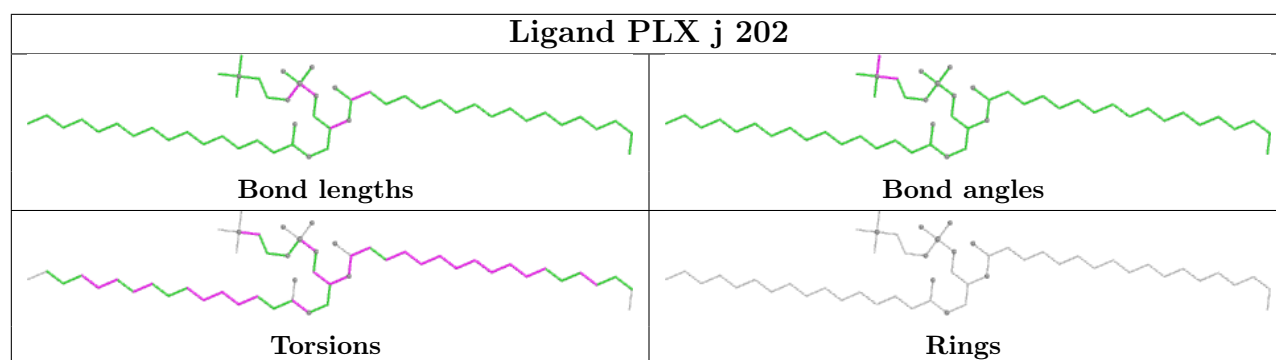


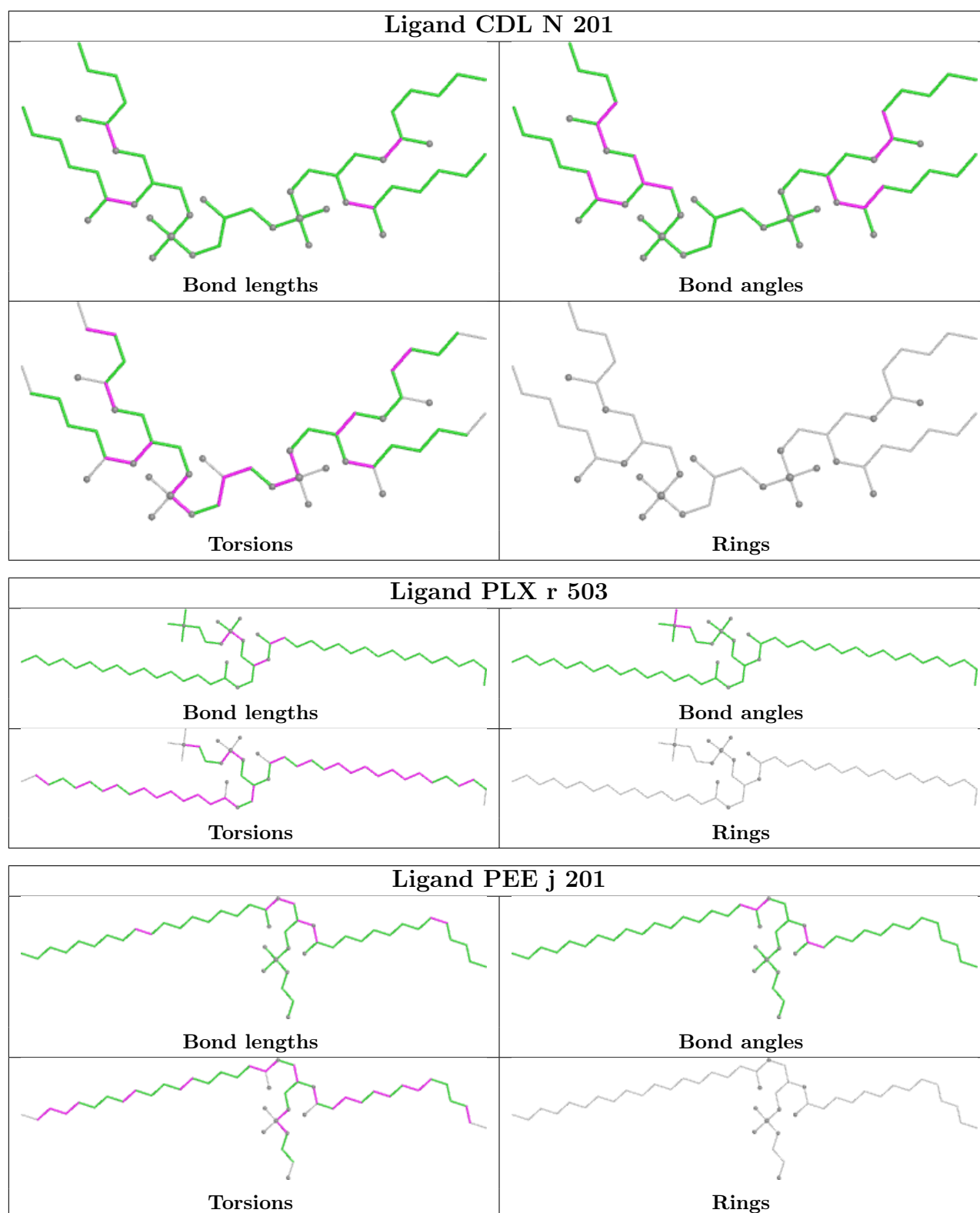












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

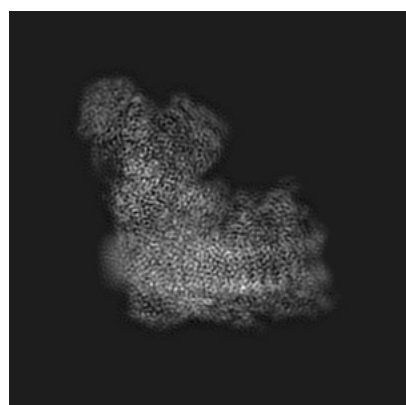
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31650. These allow visual inspection of the internal detail of the map and identification of artifacts.

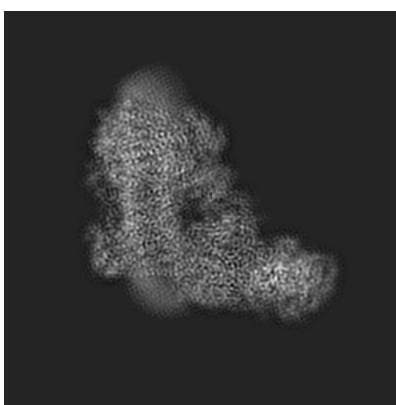
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

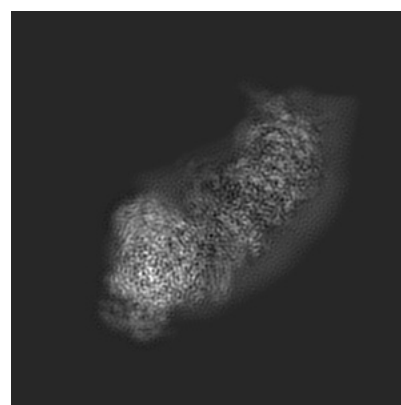
6.1.1 Primary map



X



Y

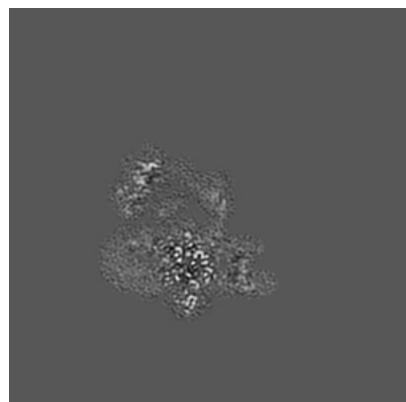


Z

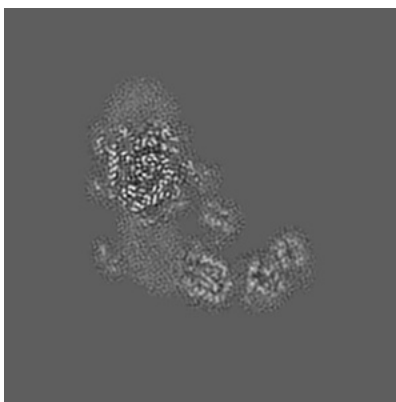
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

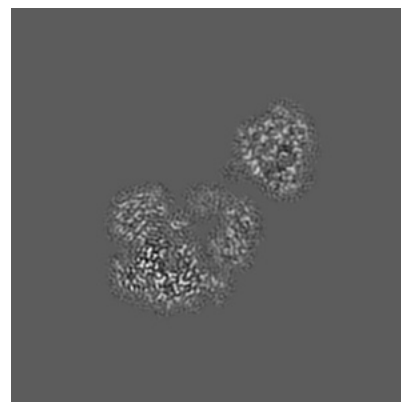
6.2.1 Primary map



X Index: 155



Y Index: 155



Z Index: 155

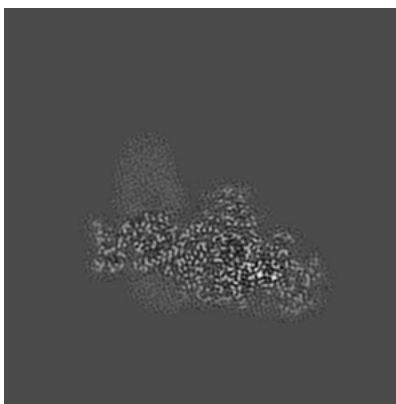
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

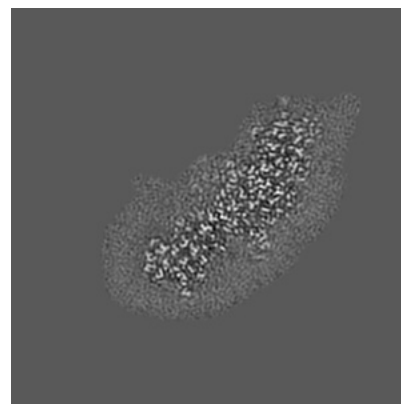
6.3.1 Primary map



X Index: 108



Y Index: 103

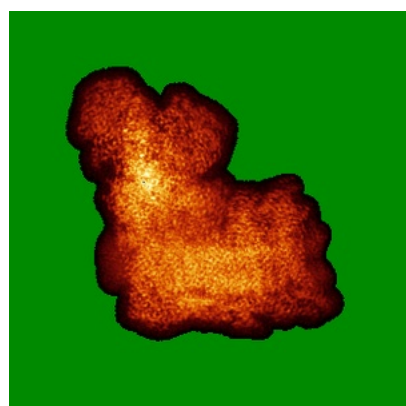


Z Index: 120

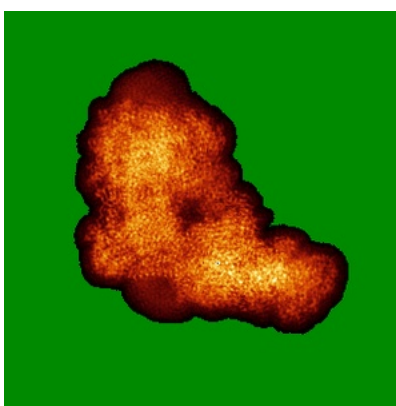
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

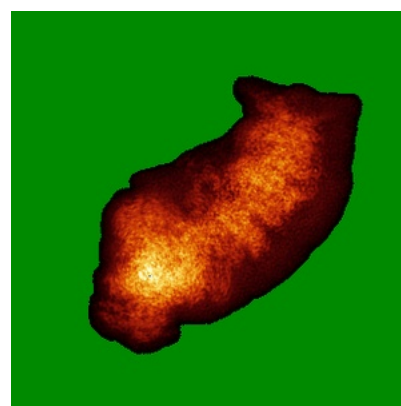
6.4.1 Primary map



X



Y

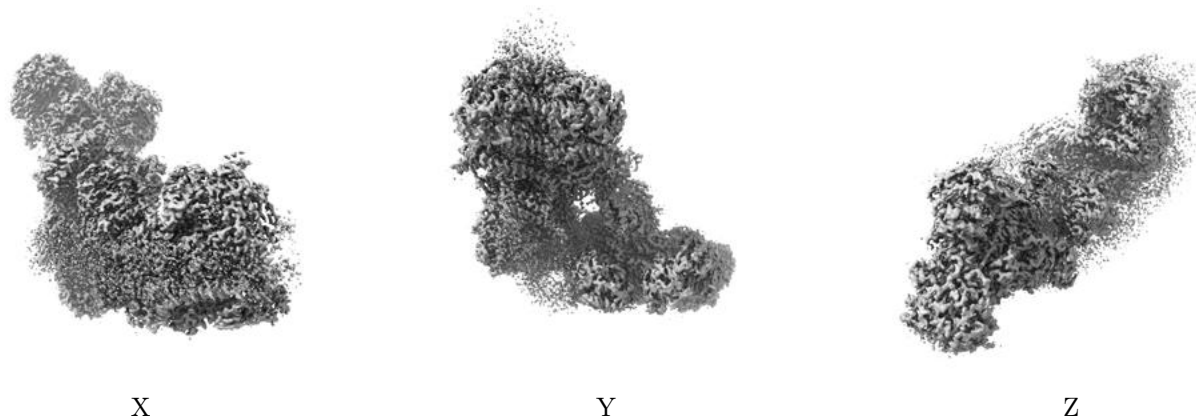


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0222. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

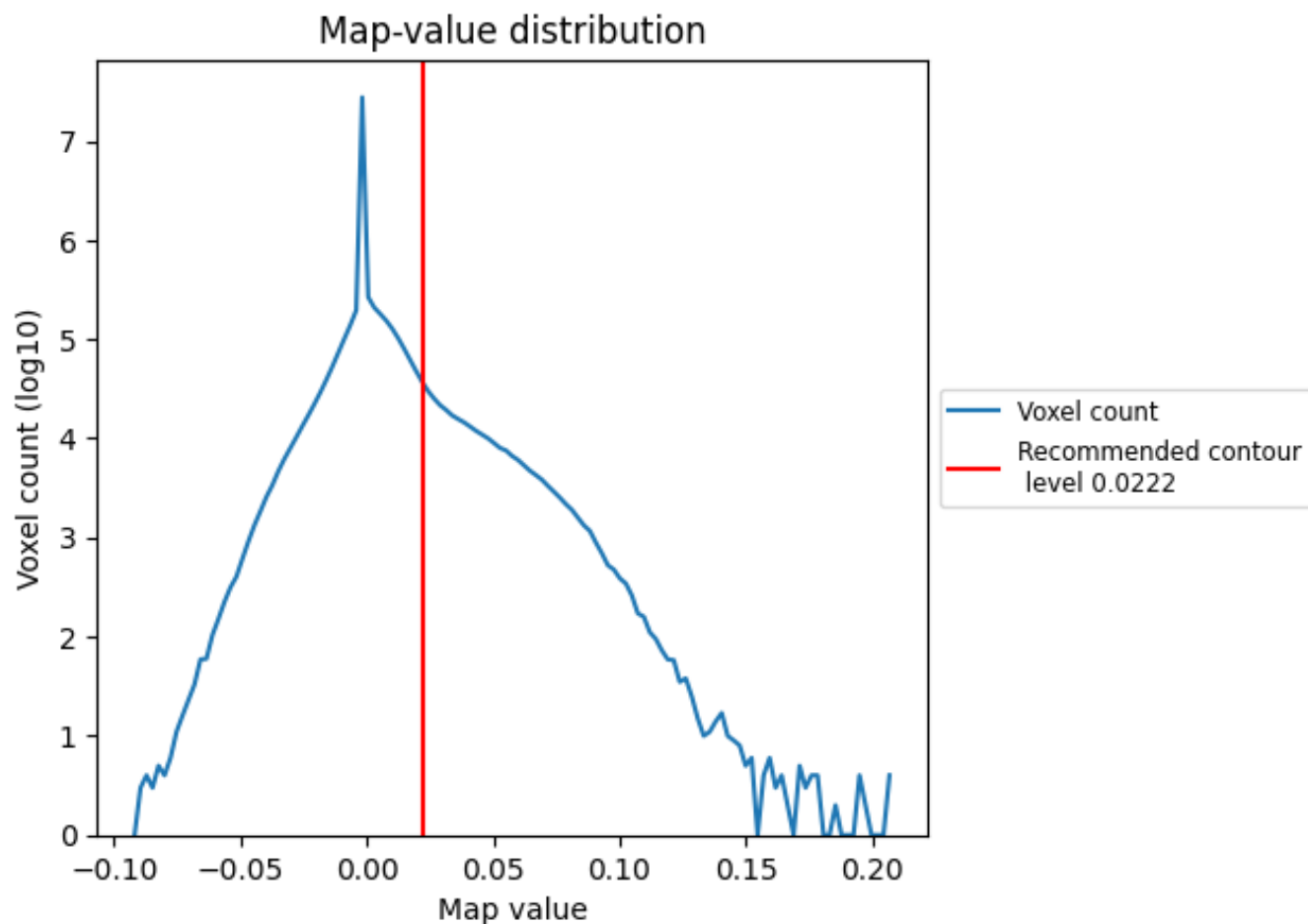
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

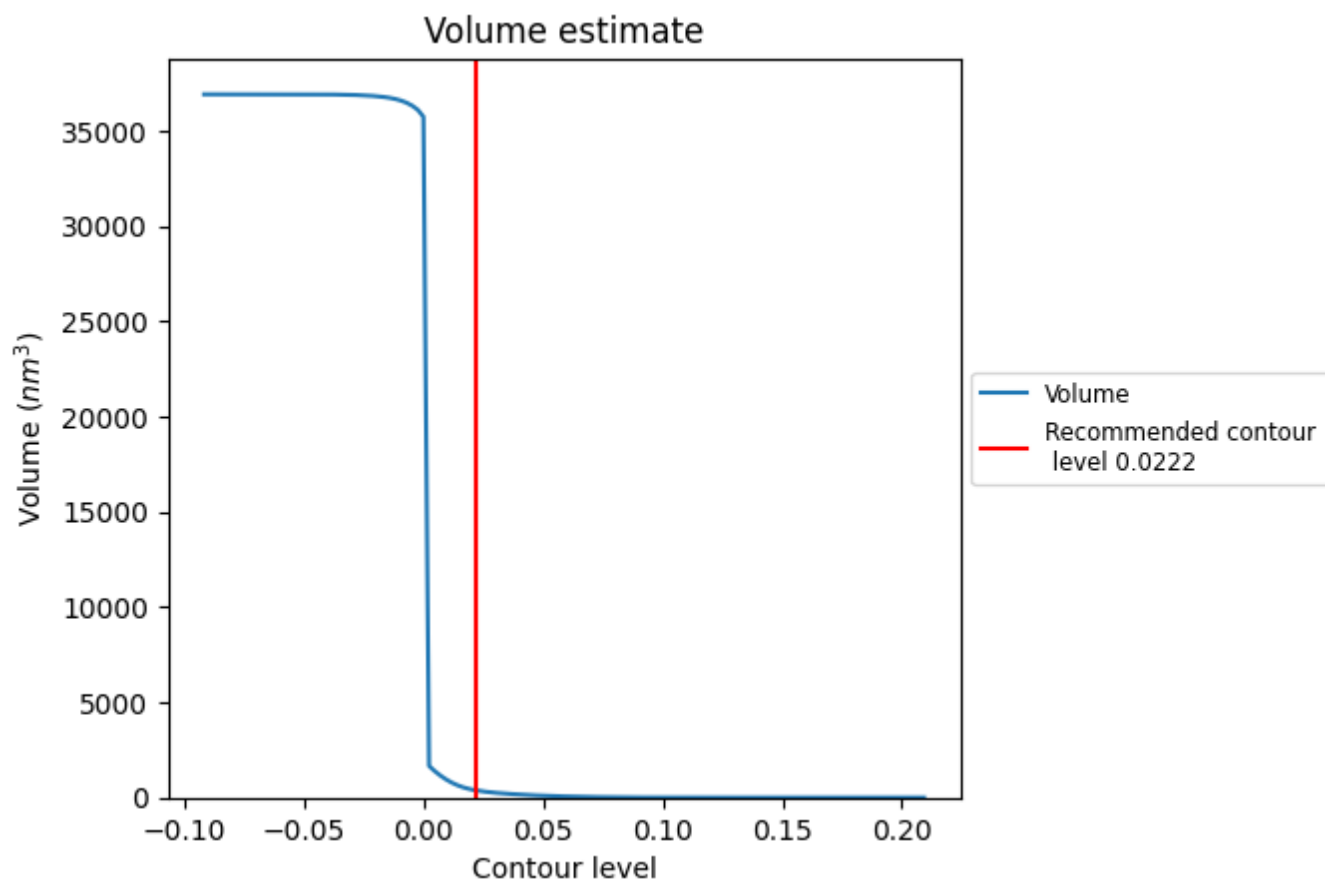
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

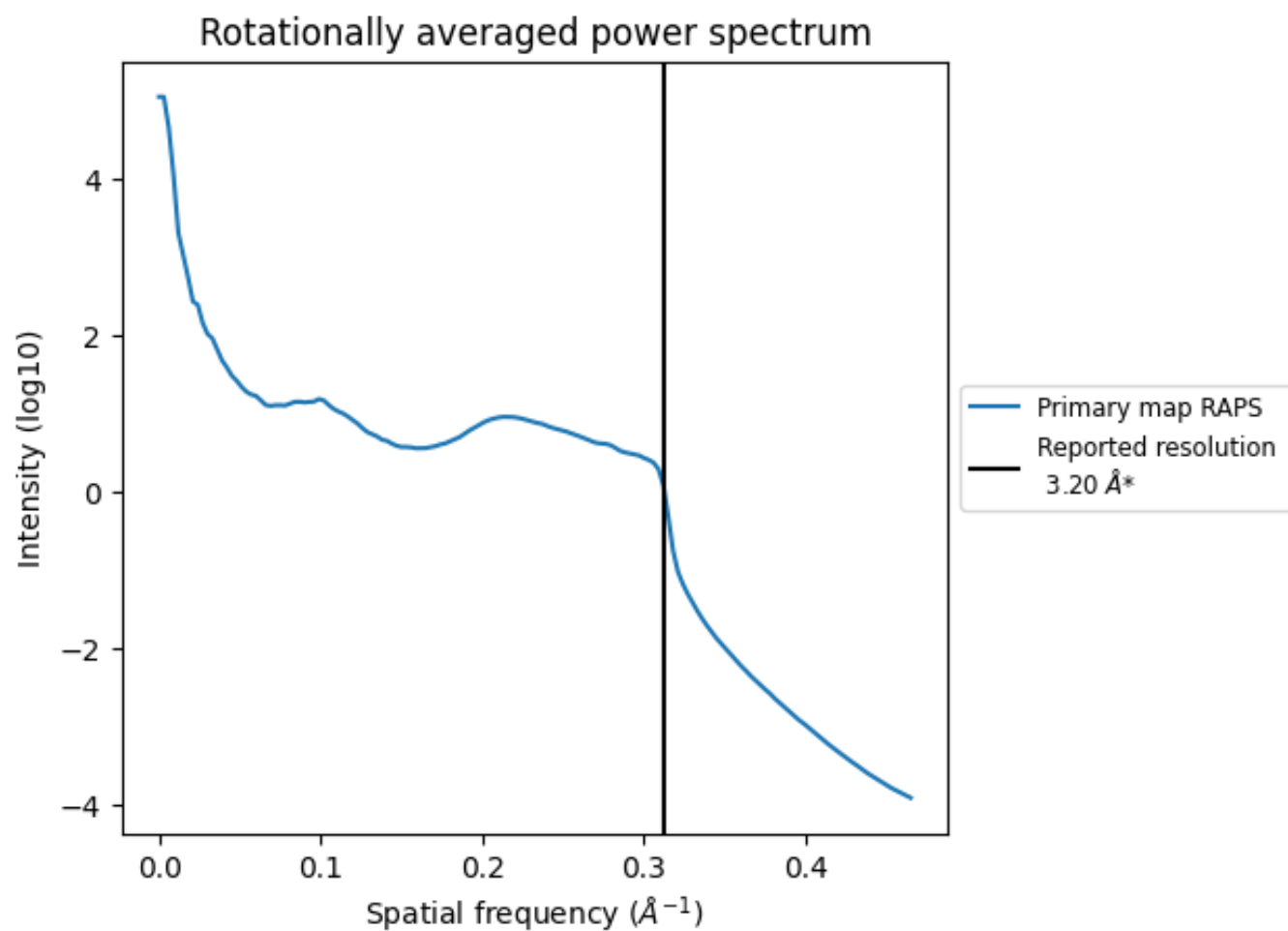
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 371 nm³; this corresponds to an approximate mass of 335 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

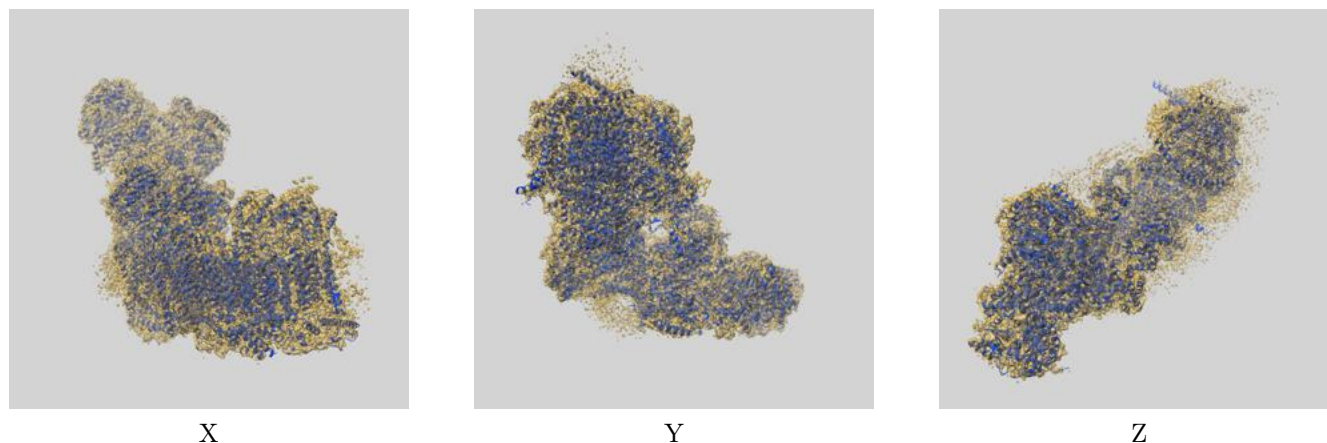
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

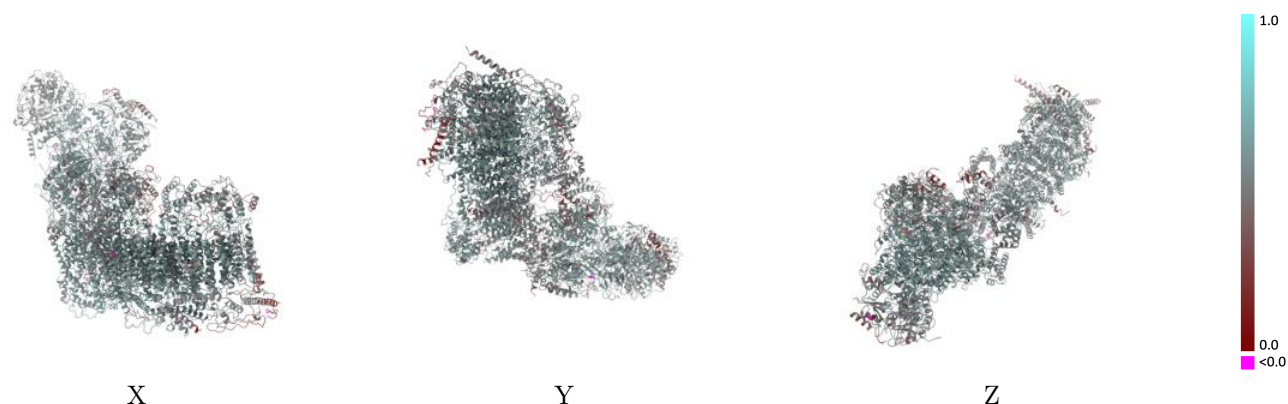
This section contains information regarding the fit between EMDB map EMD-31650 and PDB model 7V32. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

9.1 Map-model overlay [i](#)



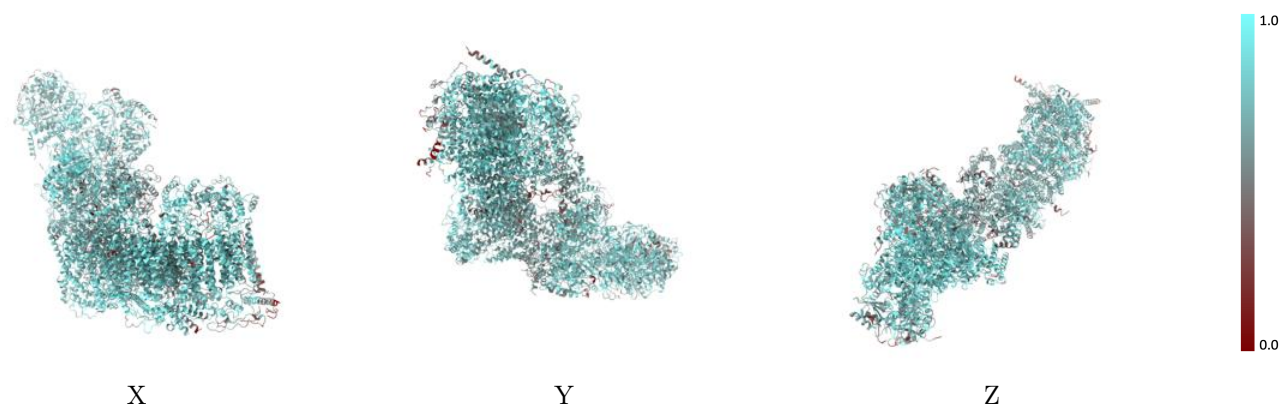
The images above show the 3D surface view of the map at the recommended contour level 0.0222 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



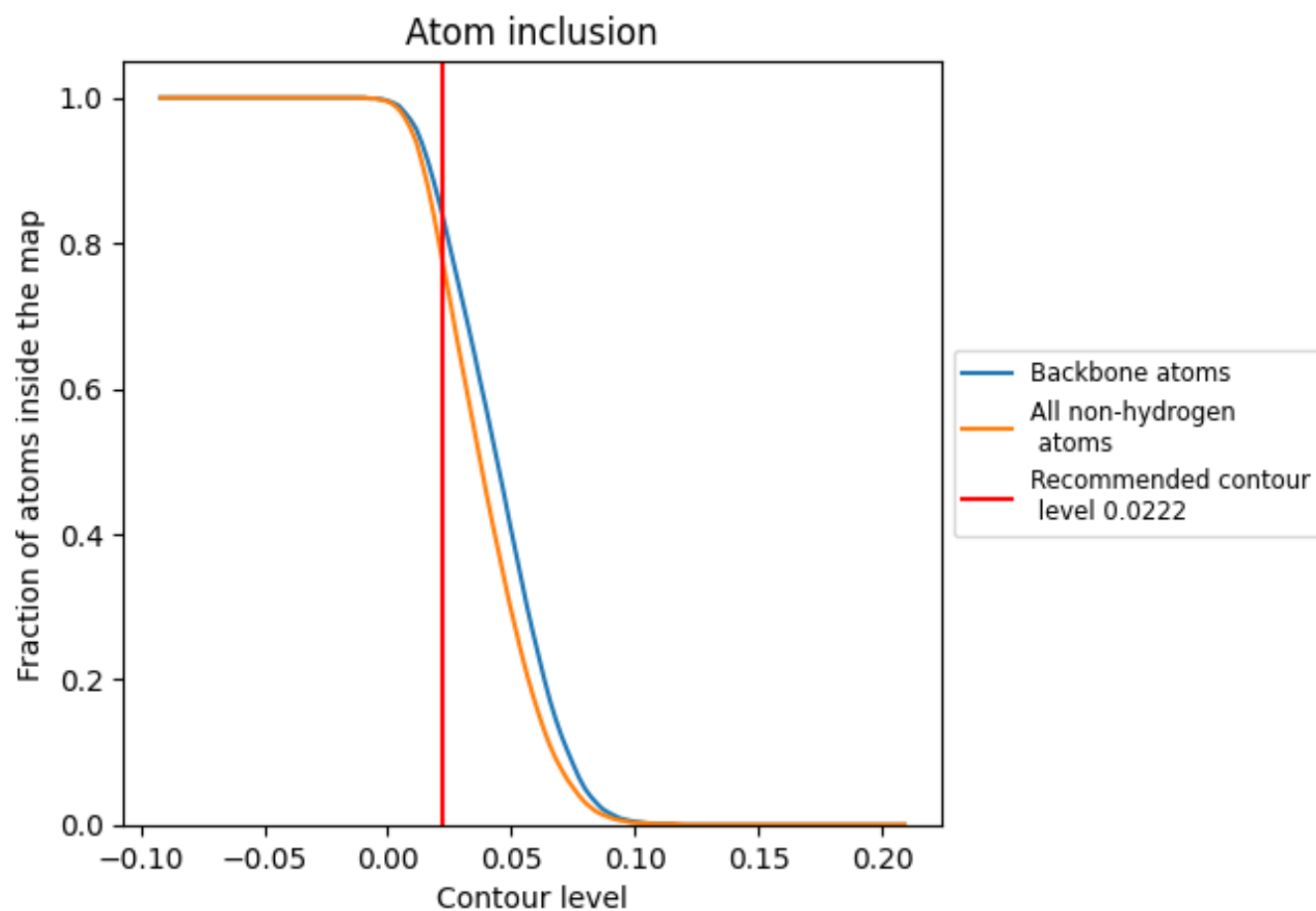
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0222).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0222) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7770	 0.5330
A	 0.7550	 0.5080
B	 0.9010	 0.5870
C	 0.8500	 0.5650
E	 0.7360	 0.5190
F	 0.6520	 0.4320
G	 0.5360	 0.4160
H	 0.7750	 0.5150
I	 0.7900	 0.5470
J	 0.7100	 0.4950
K	 0.6280	 0.4300
L	 0.8080	 0.5620
M	 0.8140	 0.5450
N	 0.7660	 0.5430
O	 0.7150	 0.4900
P	 0.8880	 0.5840
Q	 0.8510	 0.5740
S	 0.8570	 0.5660
T	 0.7050	 0.5080
U	 0.8090	 0.5400
V	 0.6120	 0.4800
W	 0.8290	 0.5550
X	 0.7050	 0.4890
Y	 0.6480	 0.4490
Z	 0.6200	 0.4600
a	 0.7990	 0.5620
b	 0.6830	 0.4800
c	 0.7610	 0.5260
d	 0.7630	 0.5200
e	 0.7150	 0.5070
f	 0.7070	 0.5040
g	 0.7990	 0.5550
h	 0.8080	 0.5500
i	 0.8440	 0.5680
j	 0.6760	 0.5110



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Chain	Atom inclusion	Q-score
k	 0.7520	 0.5390
l	 0.7860	 0.5500
m	 0.7200	 0.5180
n	 0.6760	 0.5020
o	 0.7790	 0.5300
p	 0.7810	 0.5250
r	 0.8550	 0.5750
s	 0.8250	 0.5550
u	 0.8290	 0.5570
v	 0.6350	 0.4280
w	 0.7120	 0.4990